High-order CFD and Multiscale Modelling for Aerospace and Nanotechnology Applications

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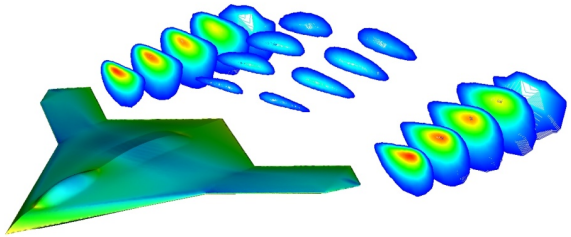
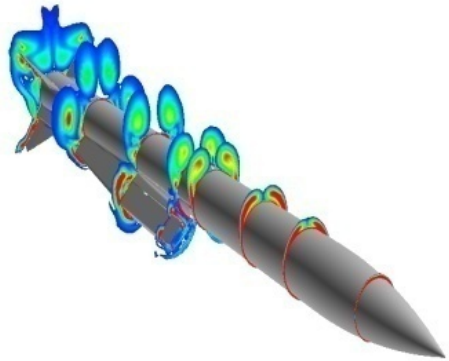
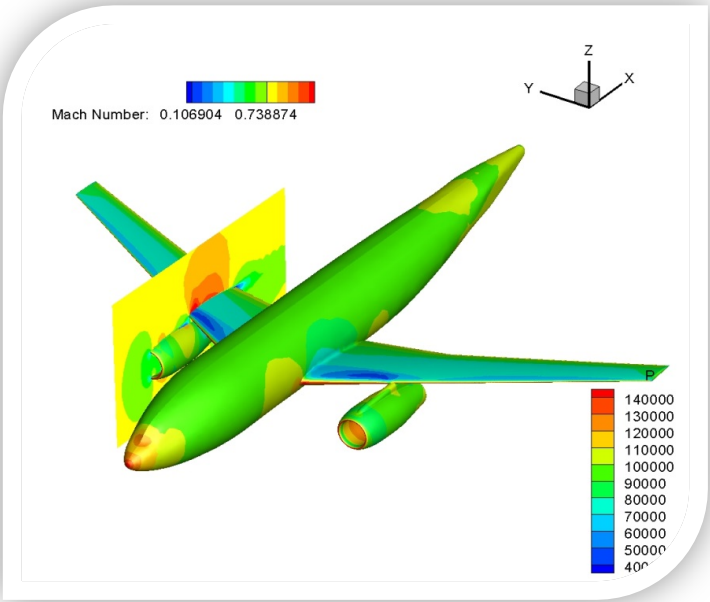
Motivation

- Advances in computational methods have increasingly enabled the simulation of complex flows, heat transfer, acoustics, and fluid-structure interaction phenomena.
- Advances in high performance computing (HPC) have allowed more complex simulations to be performed at shorter turn-around times.
- However, the design and condition monitoring of advanced aerospace systems increasingly require more detailed and accurate understanding of complex phenomena and conditions at all scales.
- Reducing the uncertainty in engineering simulations by increasing the accuracy, while making computations more efficient still remains a scientific challenge

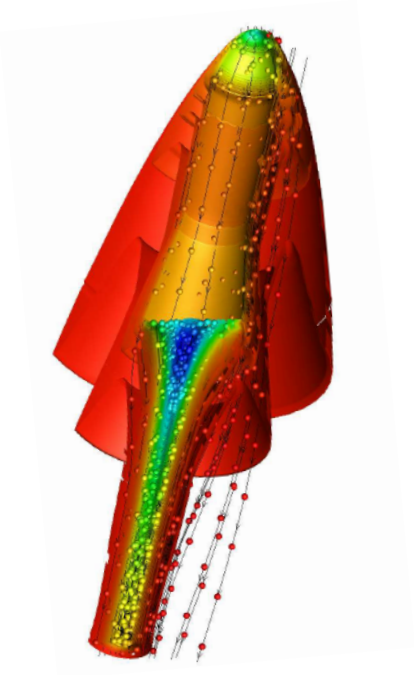




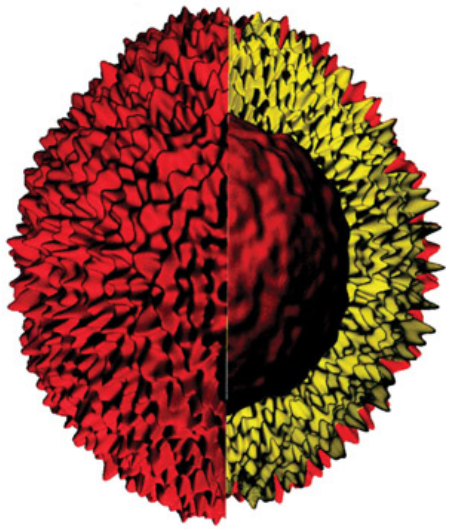
Diverse applications



Subsonic and transonic



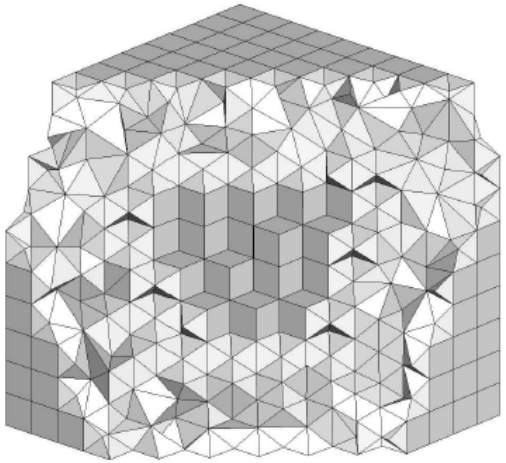
High-speed

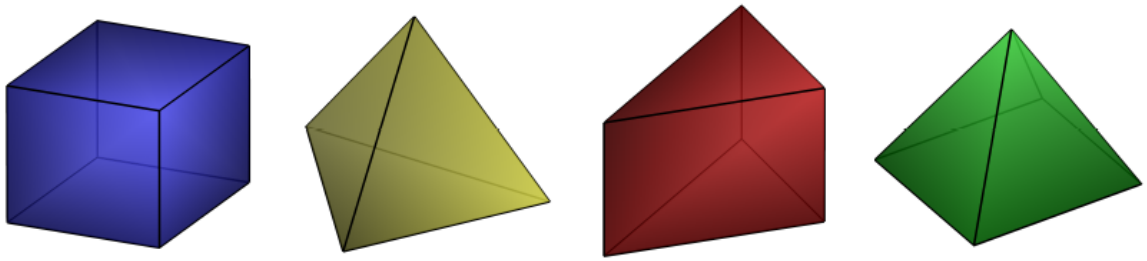


Inertial Confinement Fusion

Unstructured grids

- Consist of different types of element shapes to improve efficiency in representing complicated geometries accurately by using the minimum number of cells
- Prismatic and Hexahedral elements ideal for being used in the boundary layer region



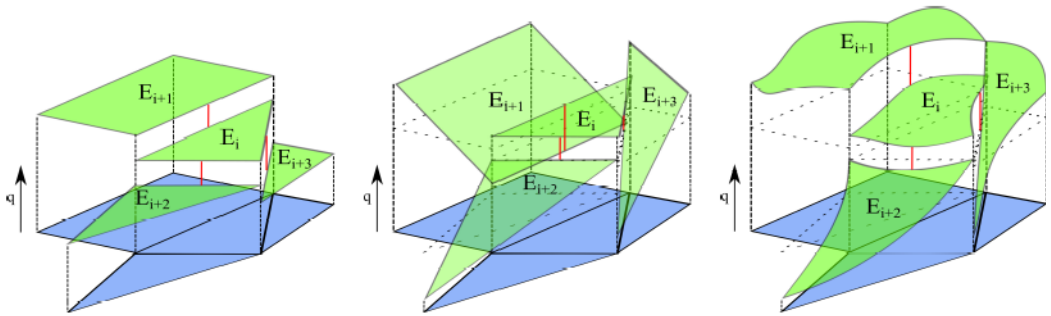


(a) Hexahedral (b) Tetrahedral (c) Prism (d) Pyramid

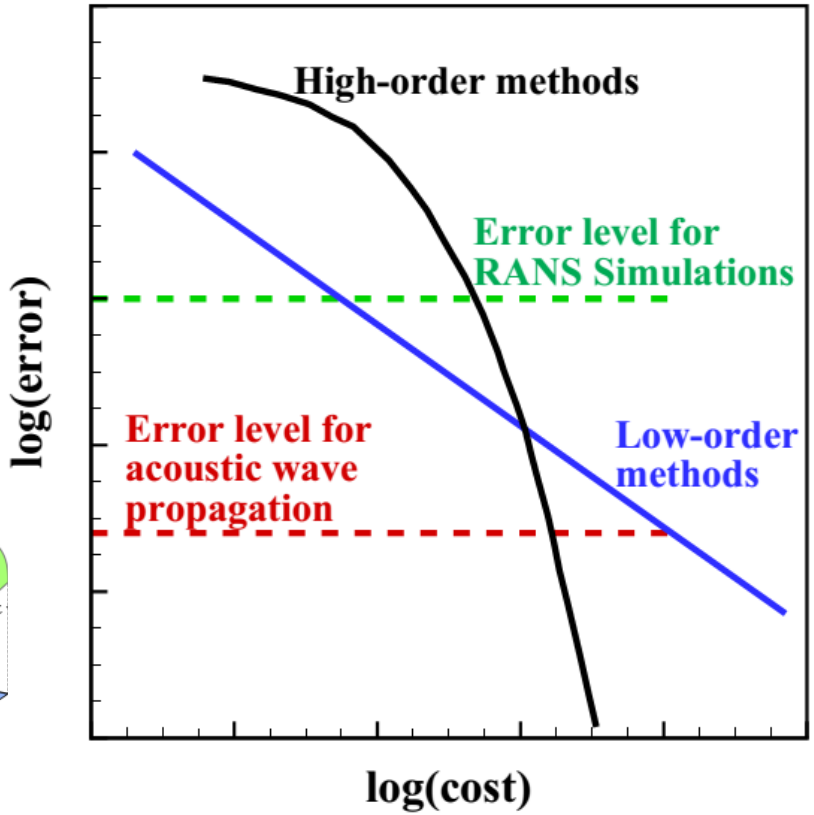
Figure 3.1: Convex polyhedrons

Spatial discretisation

- High-order of accuracy obtained by performing an interpolation (reconstruction) using the cell averages of the neighbourhood of considered cell
- Legendre type of polynomials employed for this purpose



(a) Piecewise constant 1^{st}-order (b) Piecewise linear 2^{nd}-order (c) Piecewise non-linear higher-order



Error vs cost for high and low-order methods

Low Mach Corrections

Example: Compressible Turbulent mixing,
Richtmyer-Meshkov instability

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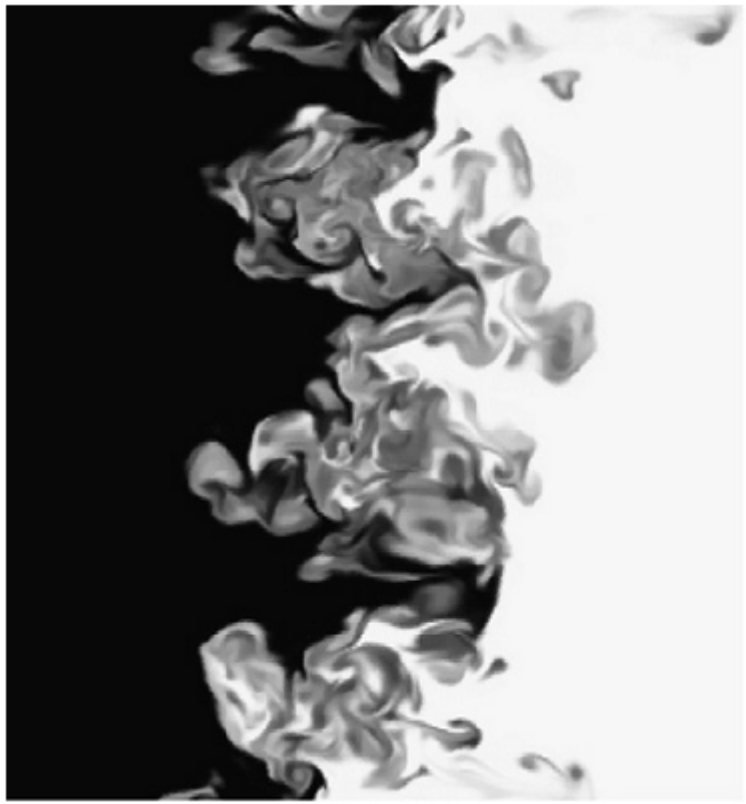
5^{th}-order method



5^{th}-order +
low Mach corrections

Effects on turbulence spectrum

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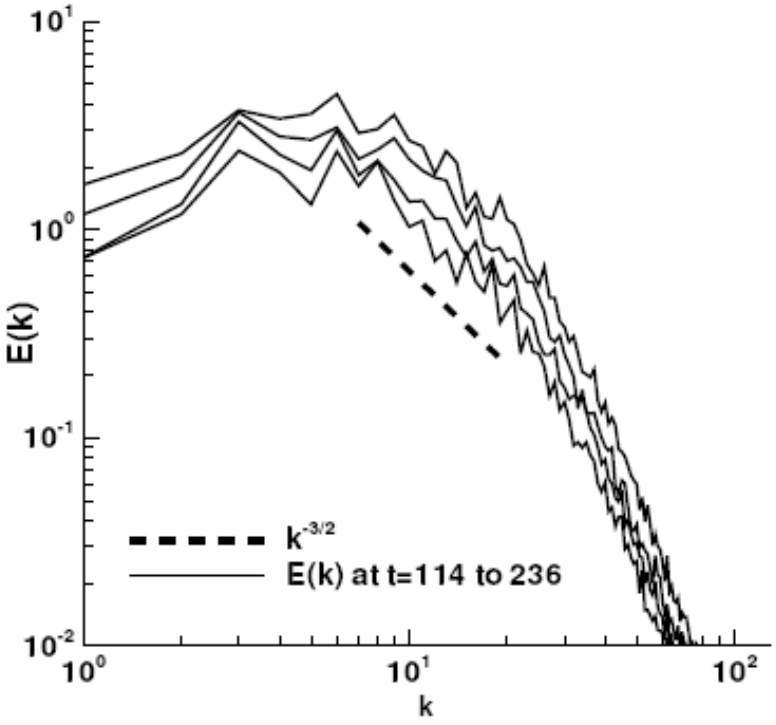
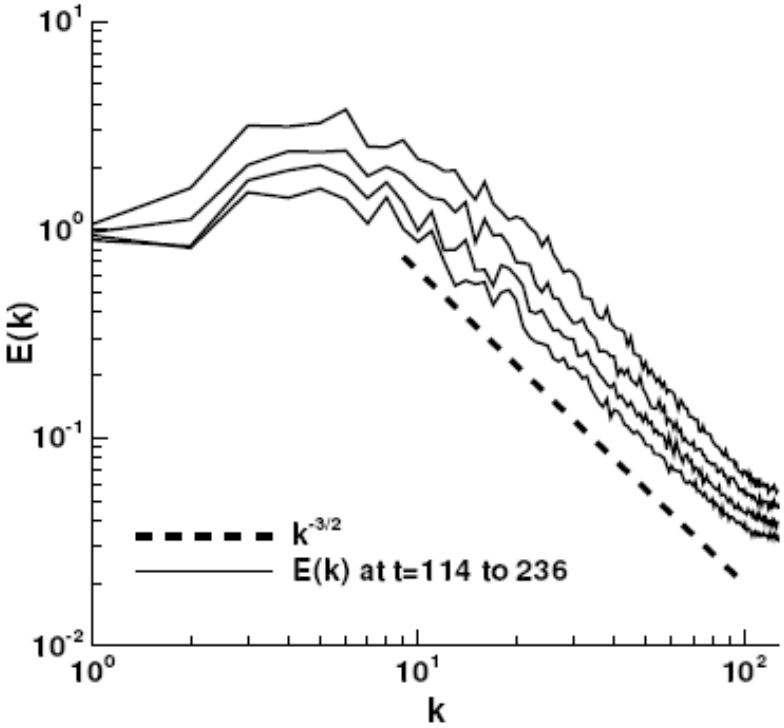
5th-order method



5th-order +
low Mach corrections



Rationale for different Turbulence Simulation Approaches

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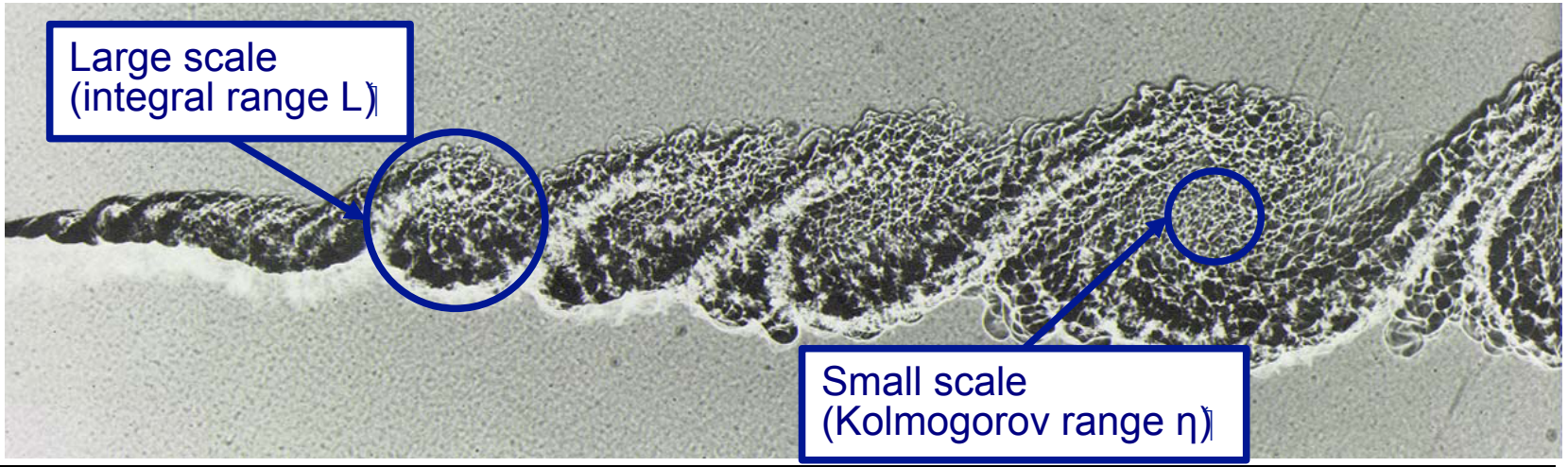
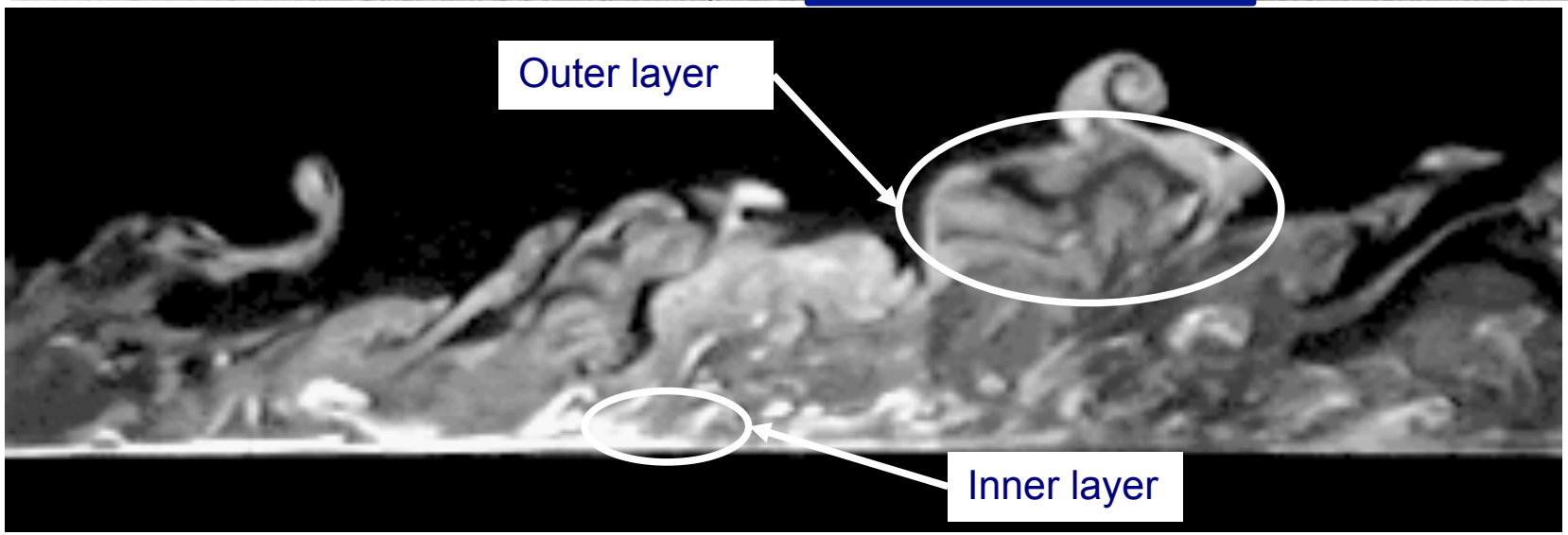
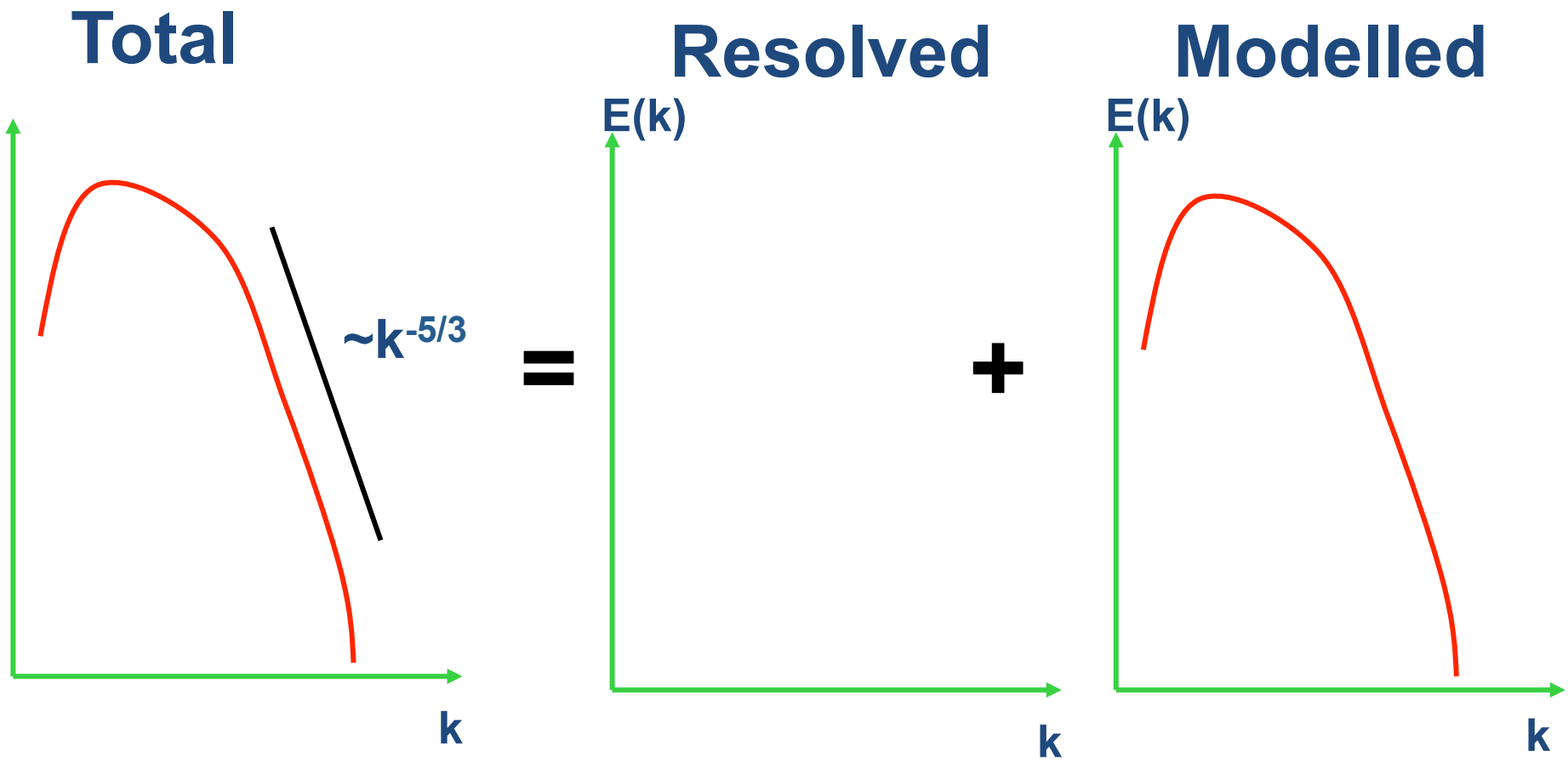
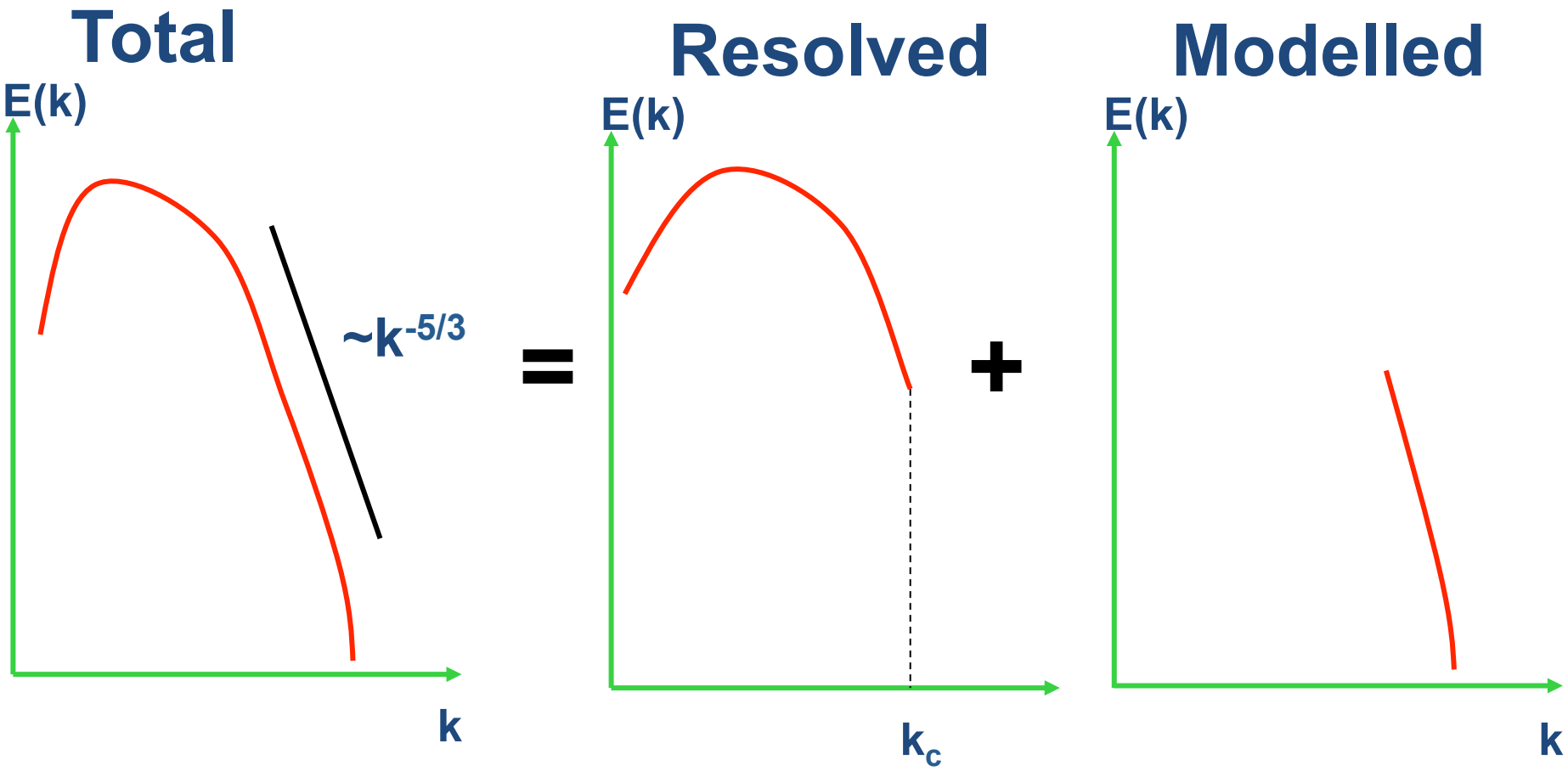




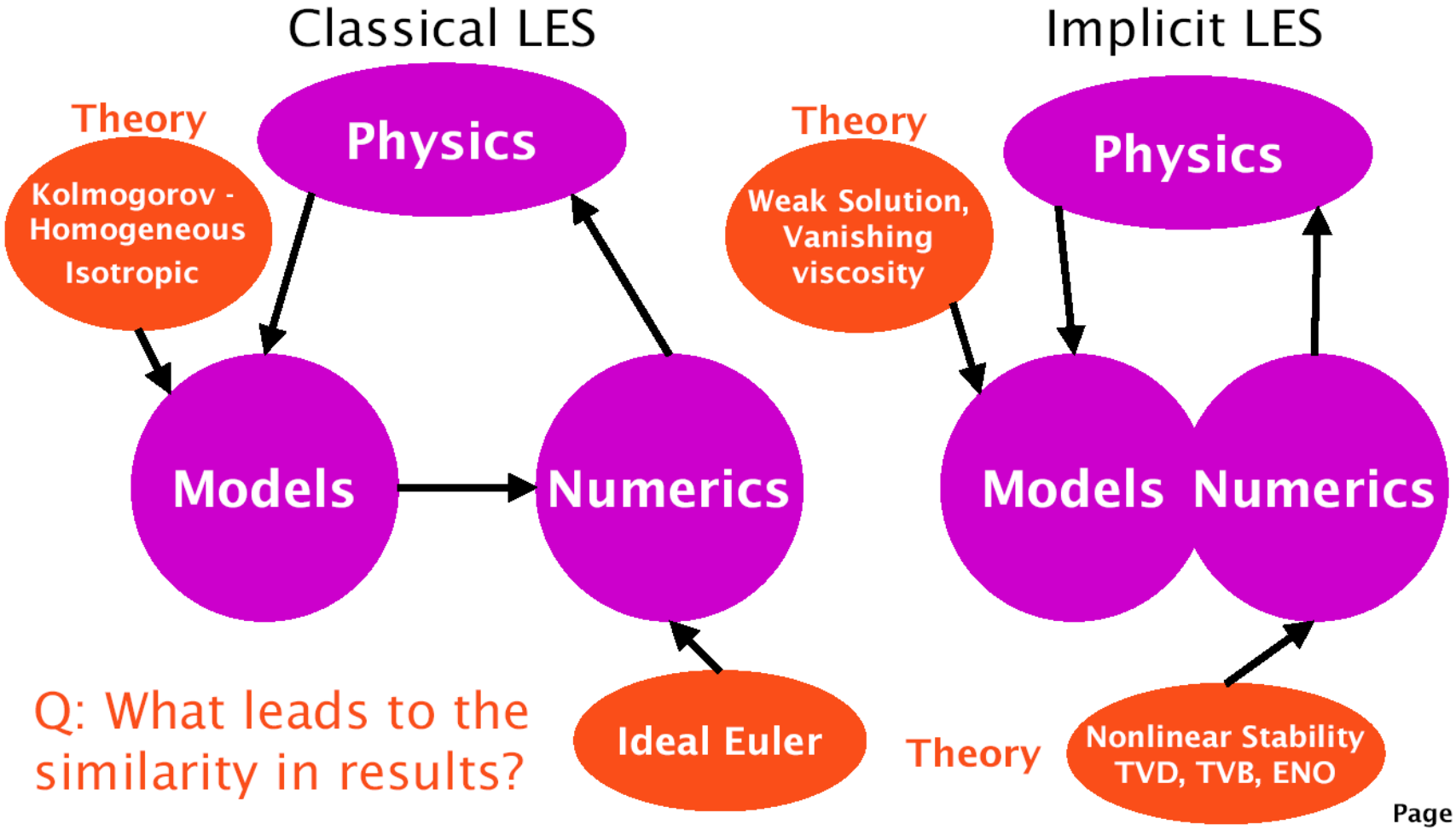
Energy cascade - Reynolds-Averaged Navier-Stokes (RANS)



Energy cascade in Large Eddy Simulation



Classical and Implicit LES



Q: What leads to the similarity in results?

Implicit & Classical Large Eddy Simulation (LES) and Detached Eddy Simulation (DES)

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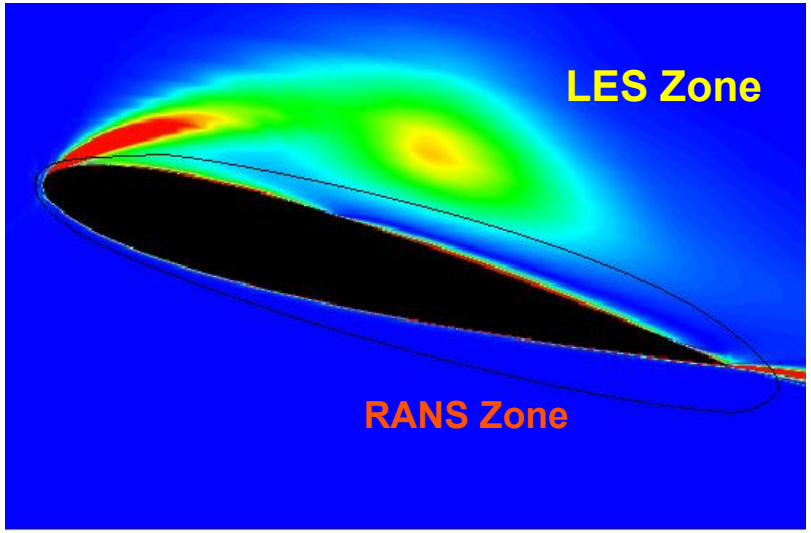
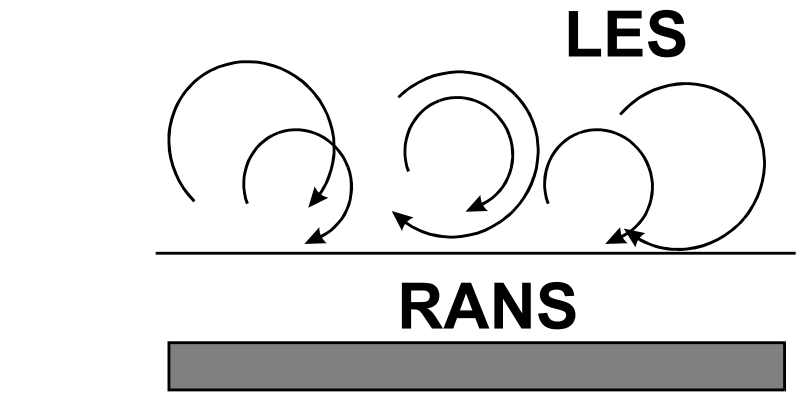
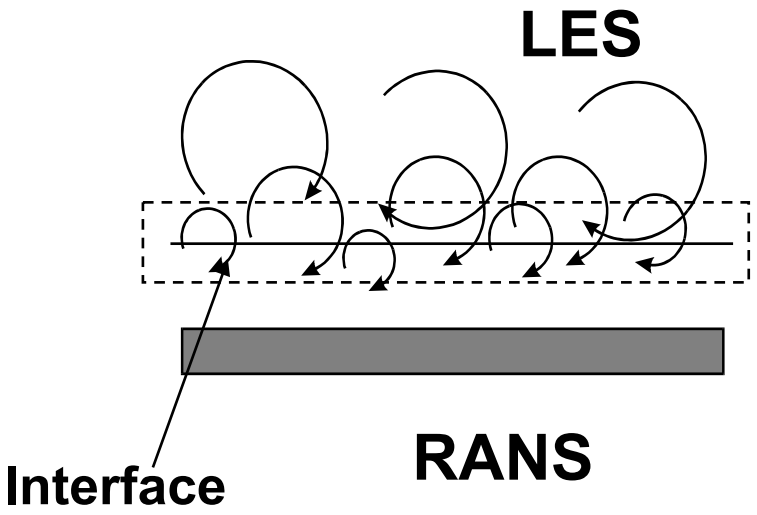
- Large Eddy Simulation
  - Implicit LES
  - Classical LES
- Detached Eddy Simulation







Computational Models – CFD Code *Azure*

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- Compressible Euler equations
- Incompressible and Compressible Navier-Stokes equations
- Reynolds Averaged Navier-Stokes equations
- Implicit Large Eddy Simulation
- Detached Eddy Simulation
- *Non-hydrostatic Euler compressible equations*

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \mathbf{divT}$$

$$\frac{\partial \rho e}{\partial t} + \nabla (\rho \mathbf{u} e) = -p \nabla \mathbf{u} + \nabla \cdot q$$

CFD Code *Azure*

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- Several Riemann solvers (HLLC, Characteristics-based, Rusanov, Roe)
- Explicit Runge-Kutta time stepping schemes from 1st to 4th order of accuracy for unsteady flow problems
- Implicit time stepping LU-SGS based on 1st-order approximate Jacobians used with local-time stepping for convergence acceleration to steady state solutions
- **RANS** with Spalart-Allmaras, K-ω (SST) turbulence models
- **Detached Eddy Simulation (DES)** or **hybrid RANS/LES** with Spalart-Allmaras and K-ω turbulence Models
- **Implicit Large Eddy Simulation (ILES)**
- RANS transport variables can be discretised in the same manner as the mean flow equations

Near wall turbulence

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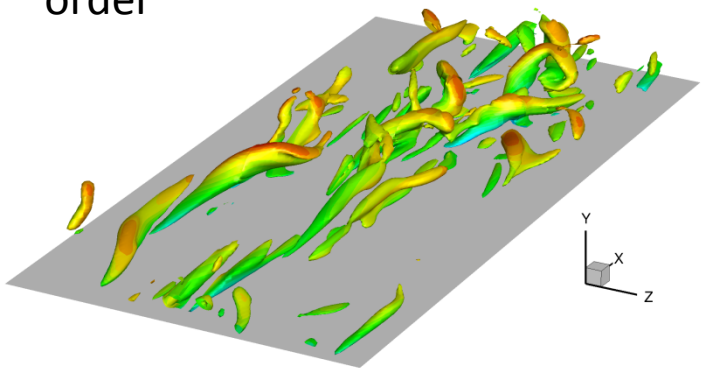
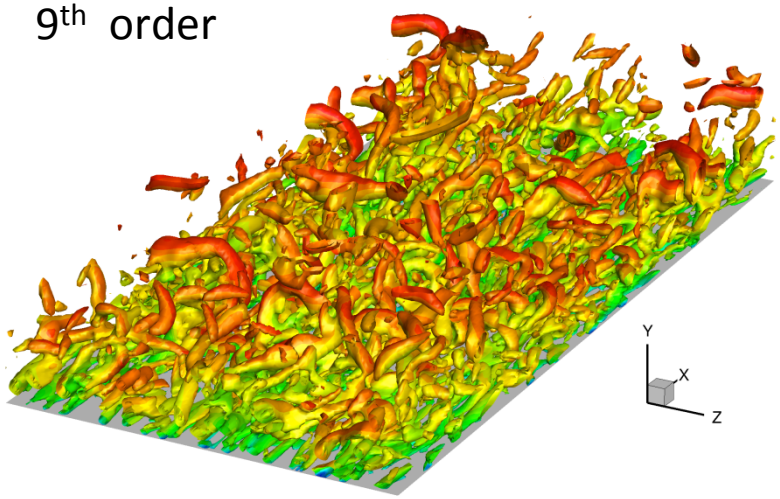
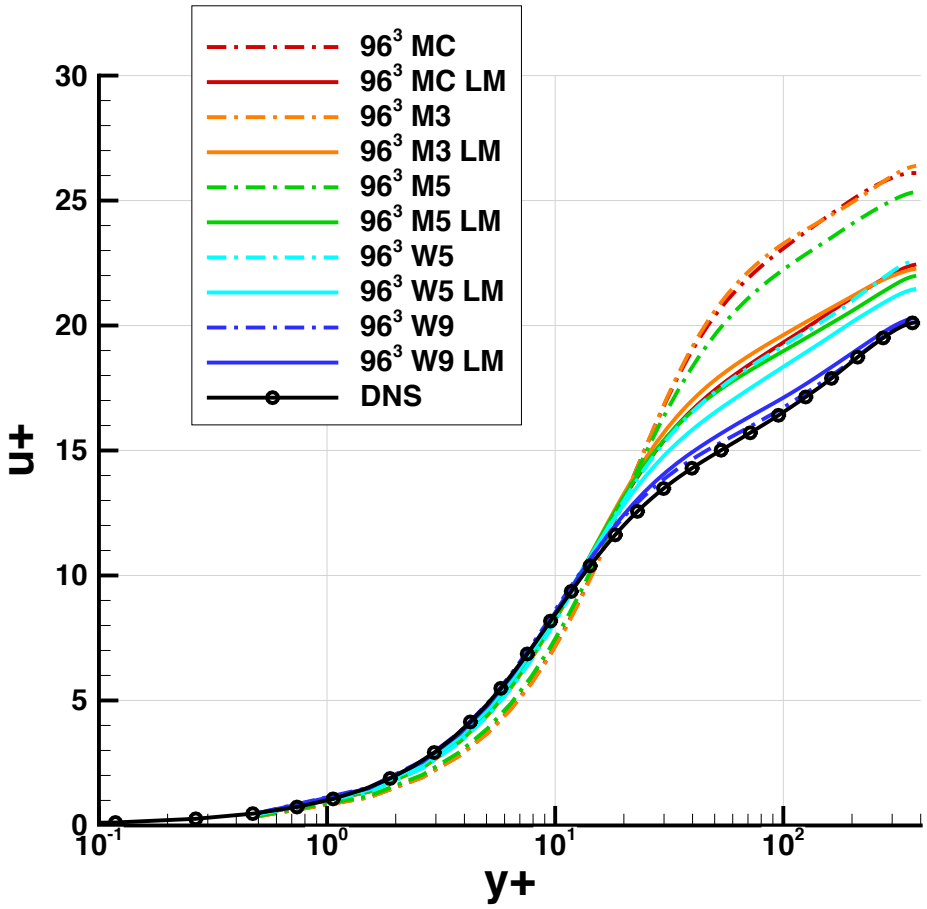
2nd order

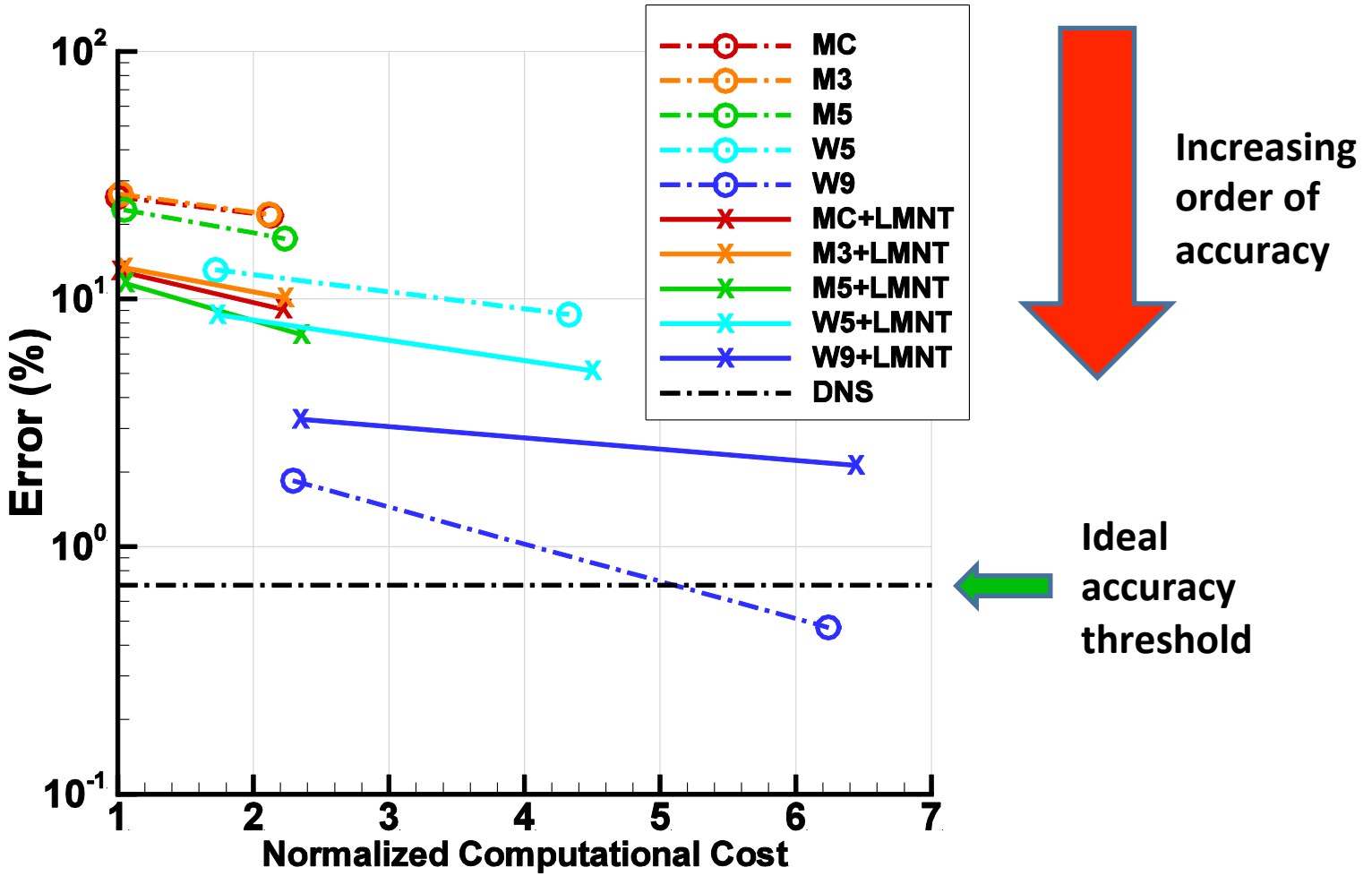


9th order





Accuracy vs computational cost



Separated flows – Swept wings

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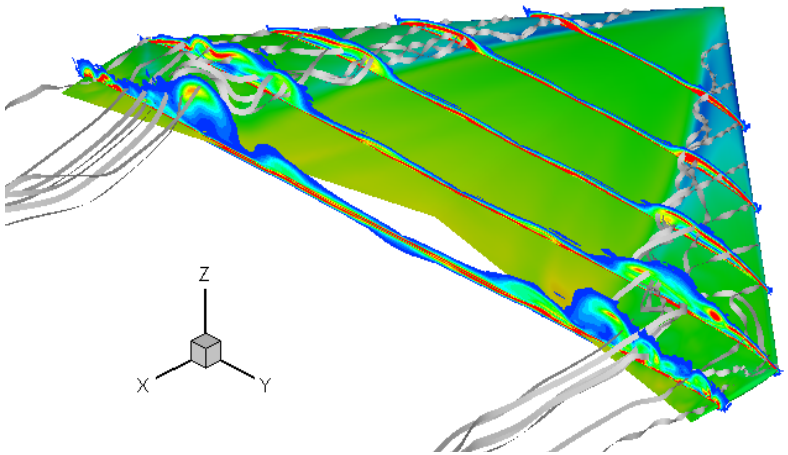
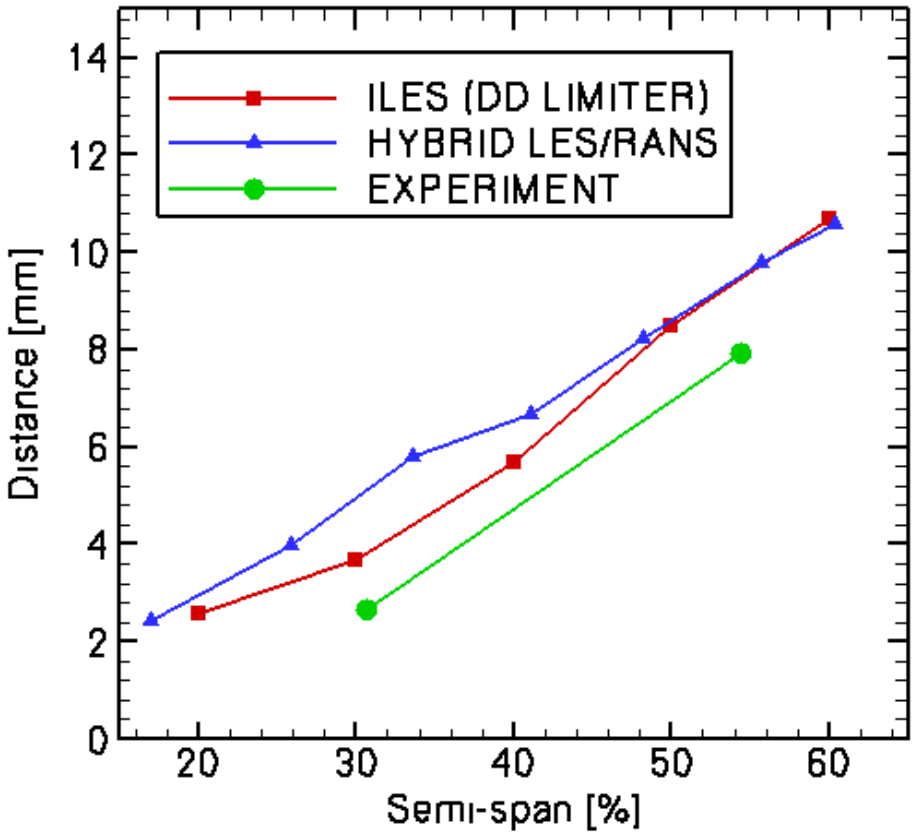
$Re=2x10^5, M=0.03$



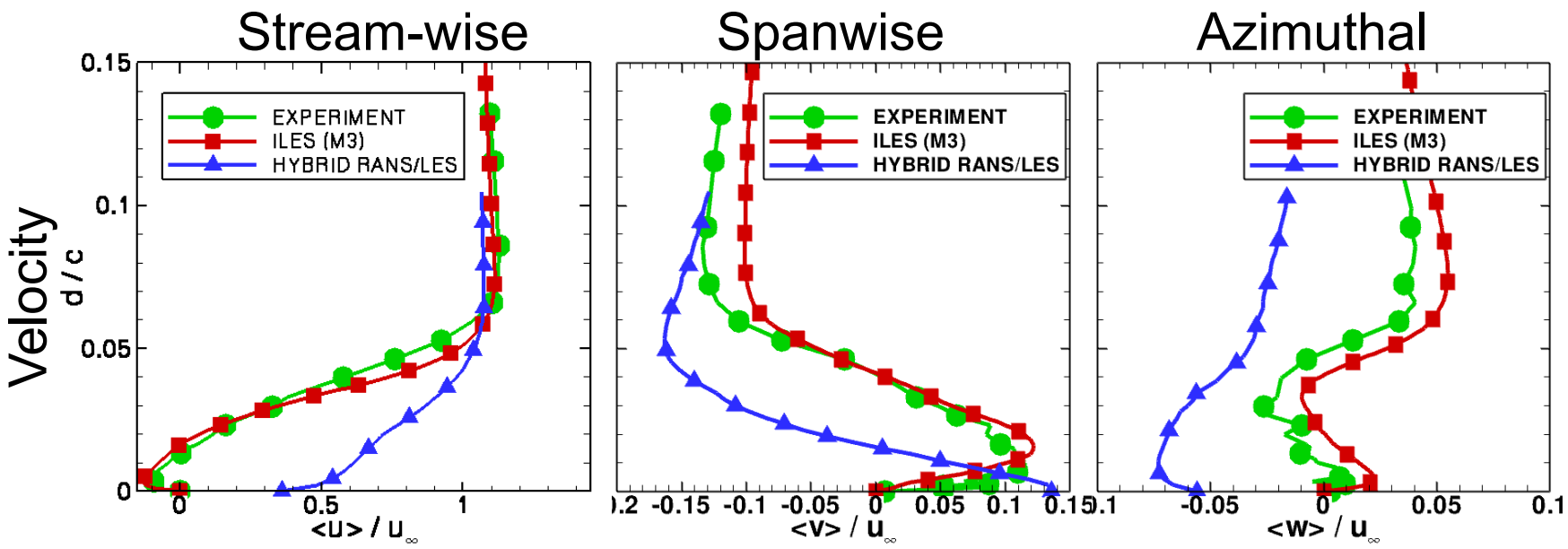
Instantaneous streamlines, vorticity and pressure

Clearance of the vortex core



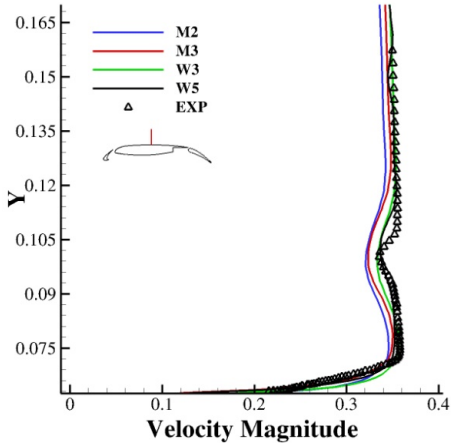
ILES vs hybrid RANS/LES

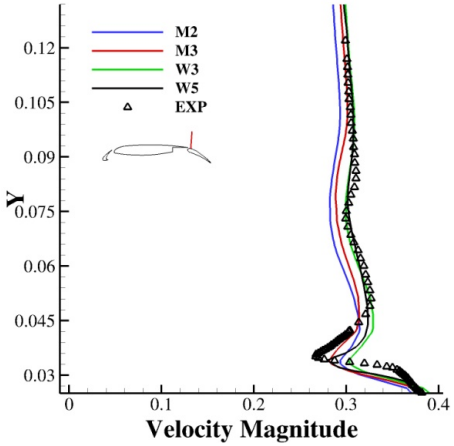
90% half-span, 50% local chord

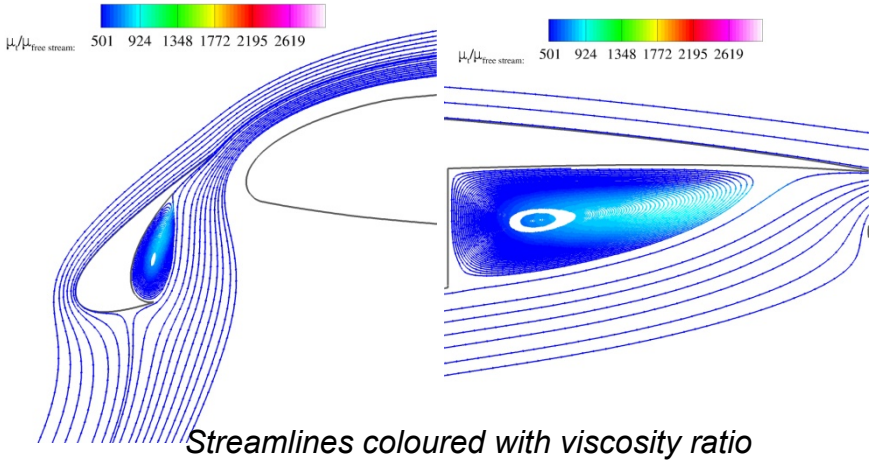


Subsonic Flows

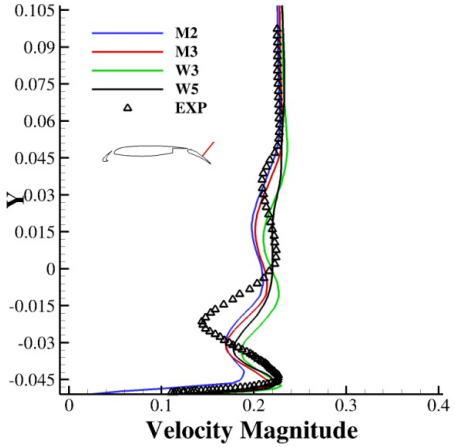
MDA 30P-30N

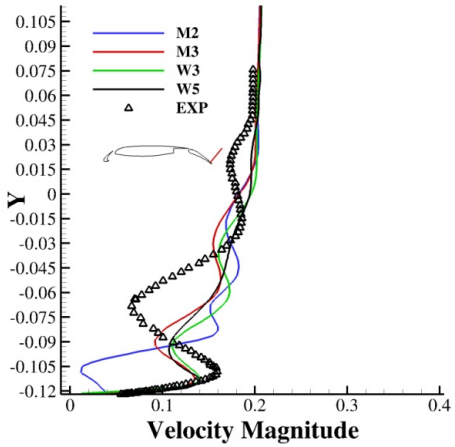


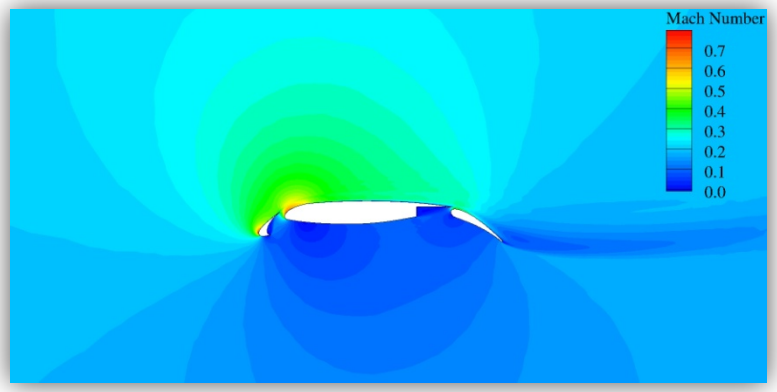




Streamlines coloured with viscosity ratio

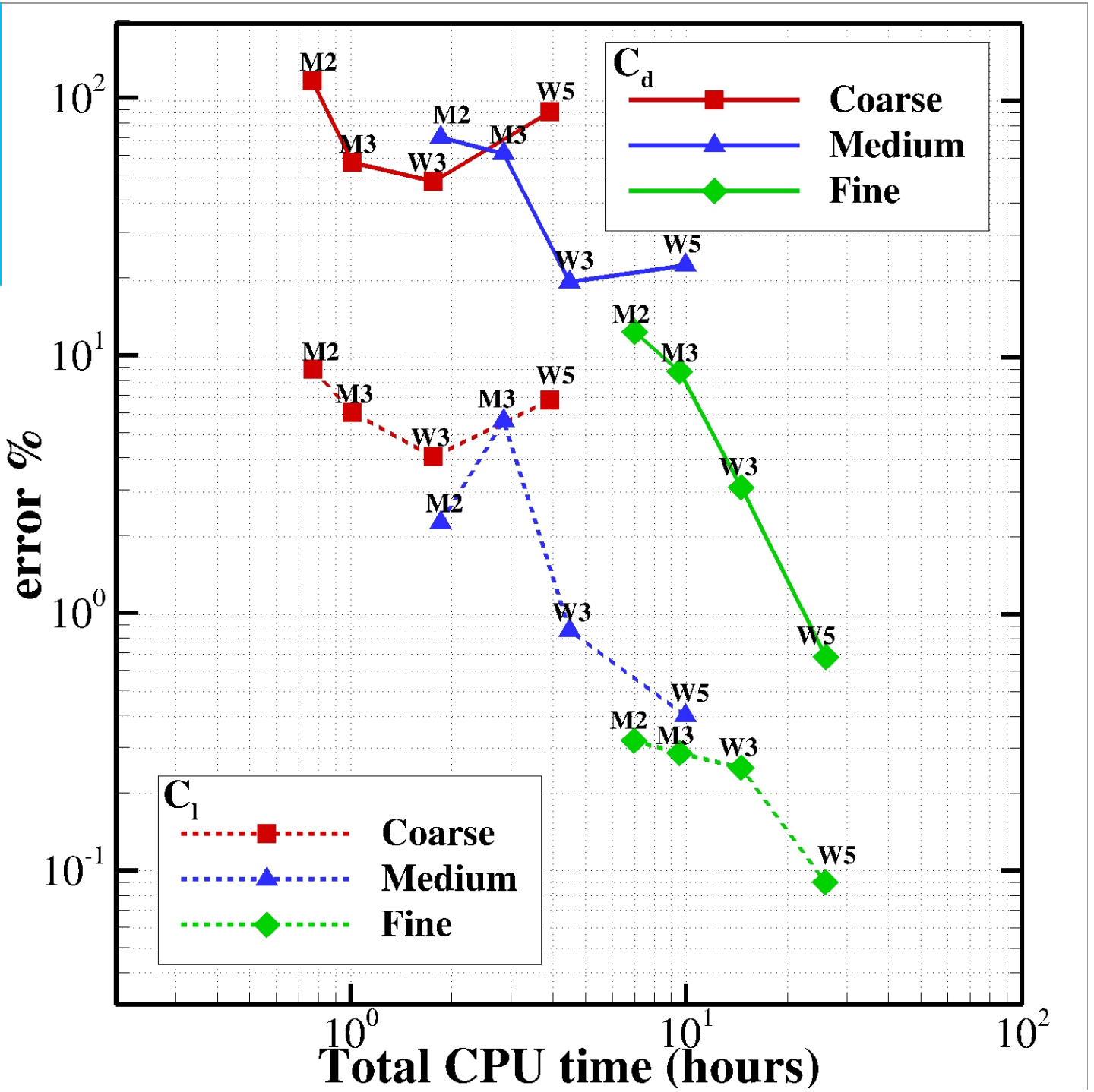






Mach number contours for the WENO 5th order

Computational efficiency vs error reduction



Transonic DLR F6 aircraft
Azure CFD code

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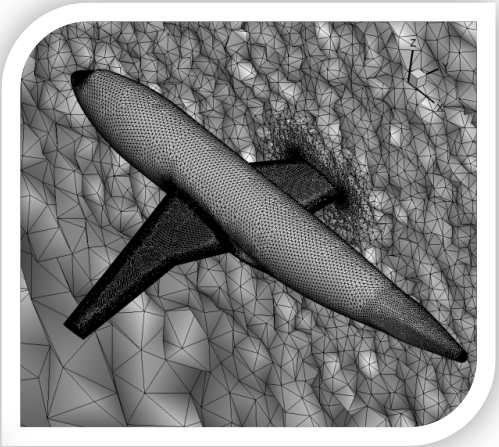
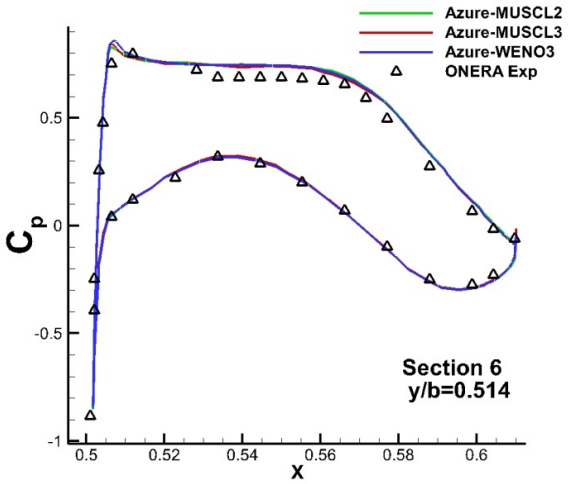
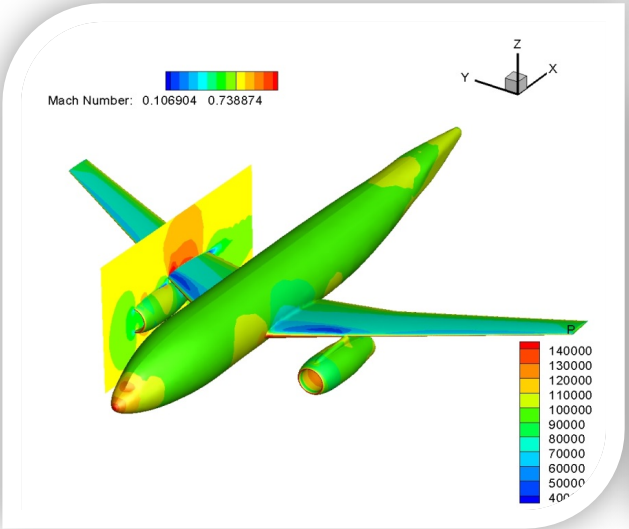
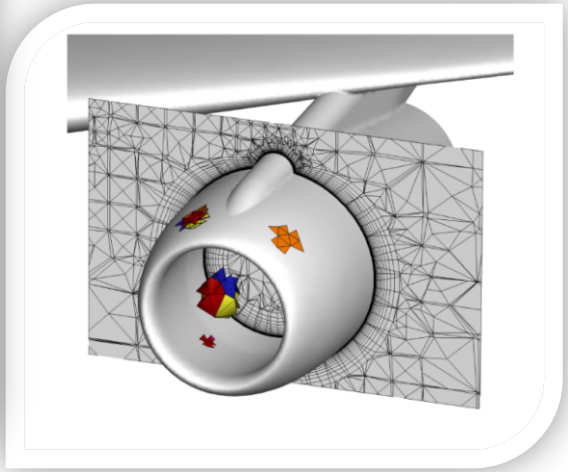
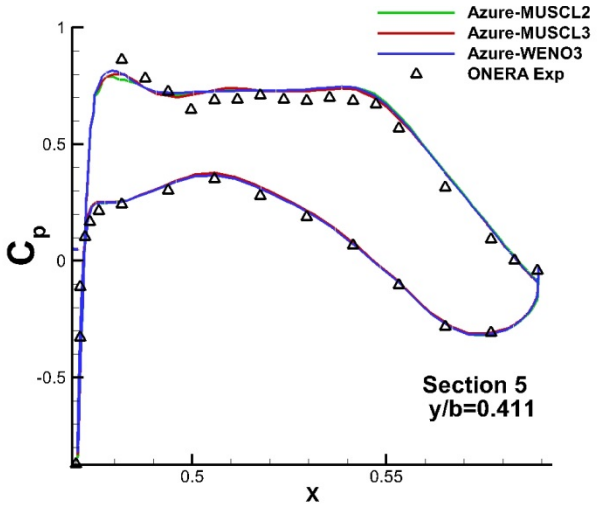
Convergence achieved in less than 17 hours for a WENO 3rd-order scheme, on one node of 16 CPUs, 5M grid points











DLR F11 aircraft – *Azure* CFD code

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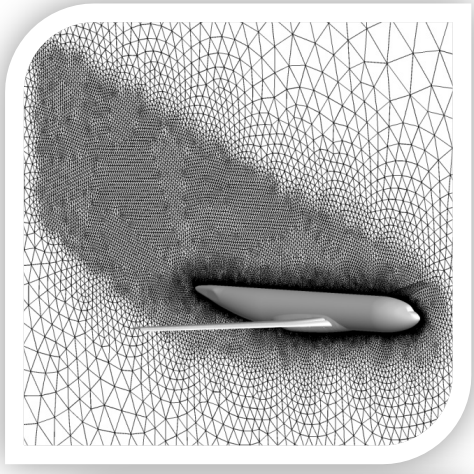

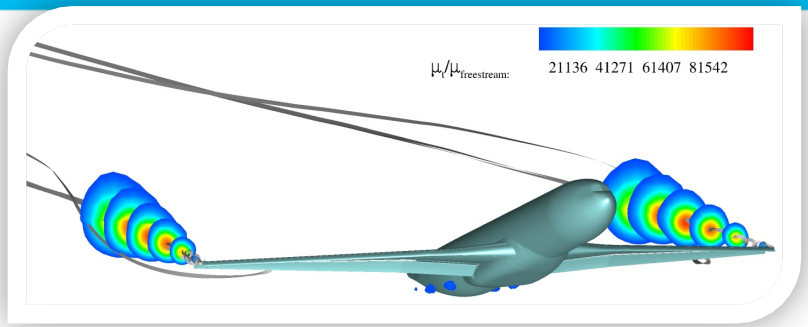

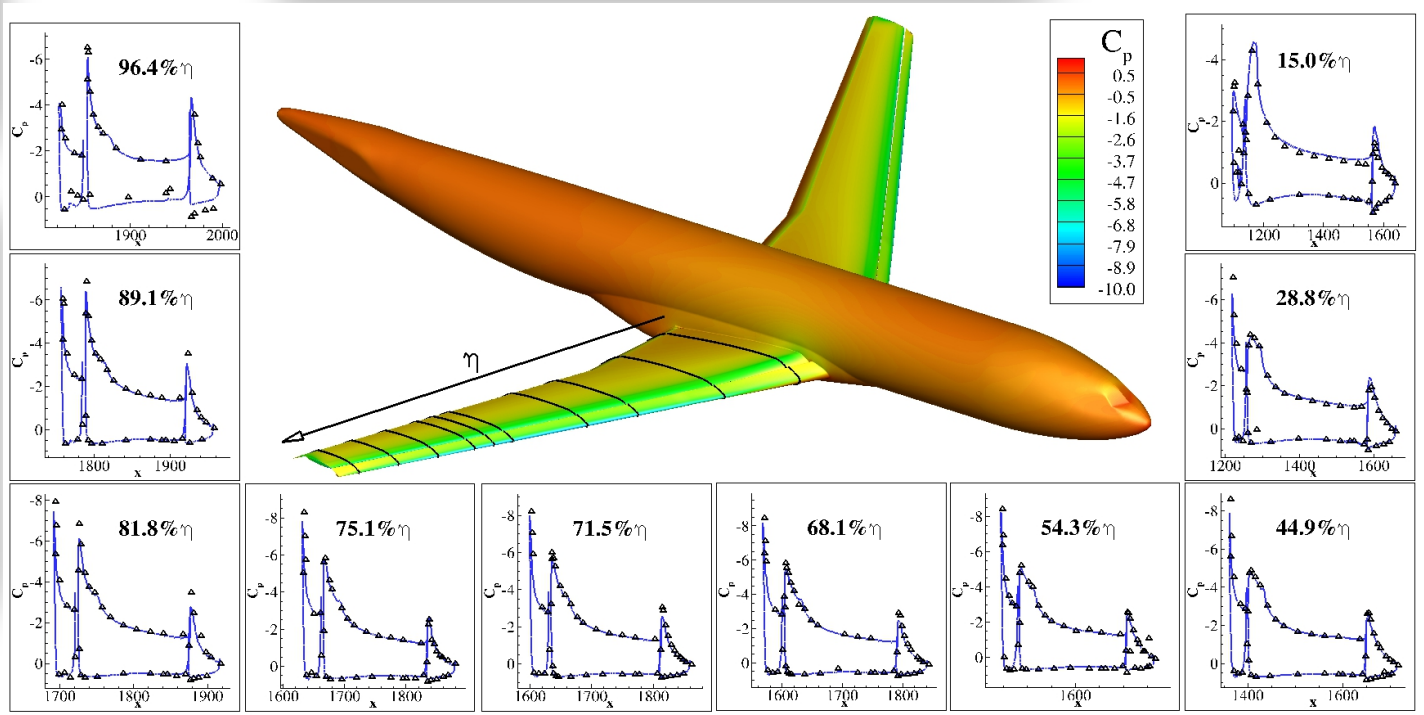

Pressure coefficient – comparison of methods

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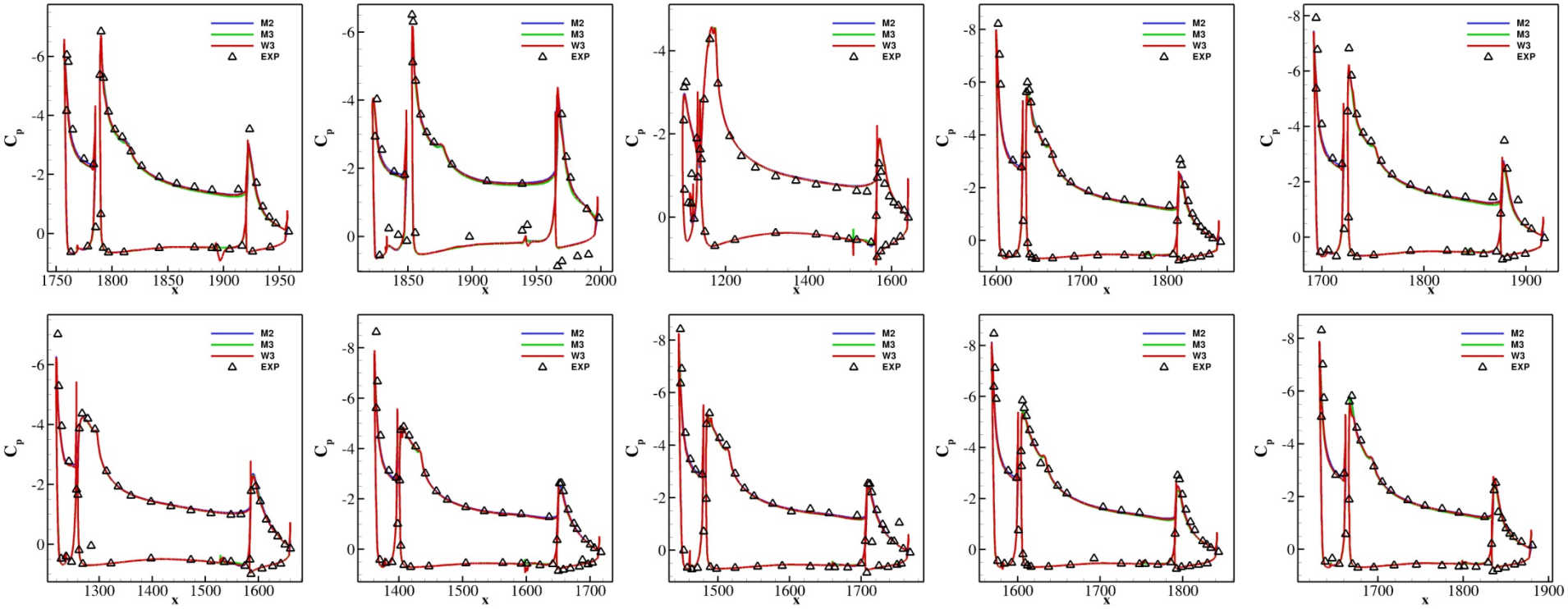
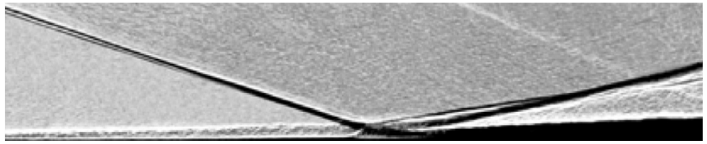
Full aircraft DLR-F11 high-lift configurations

with MUSCL 2nd, 3rd and WENO 3rd order schemes

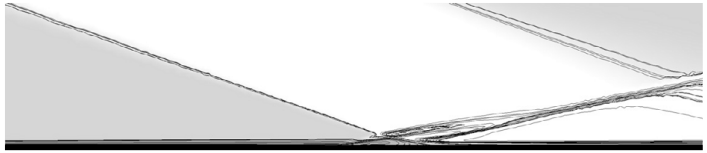


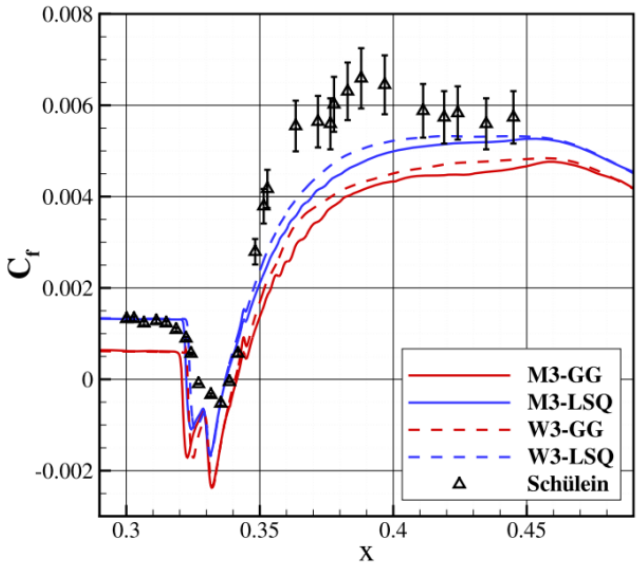
Shock wave/boundary layer interaction

- **Qualitative results showing the computed density for the WENO 3rd order scheme illustrating the shock structure compared with the shadowgraph from the experiment.**
- **Comparison of gradient reconstruction Green Gauss (GG) and least-square (LSQ) with the experimental data**

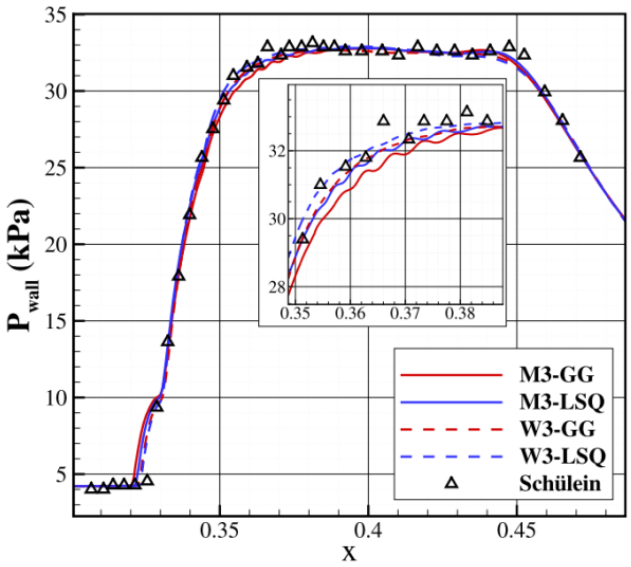


(a) Experimental shadowgraph





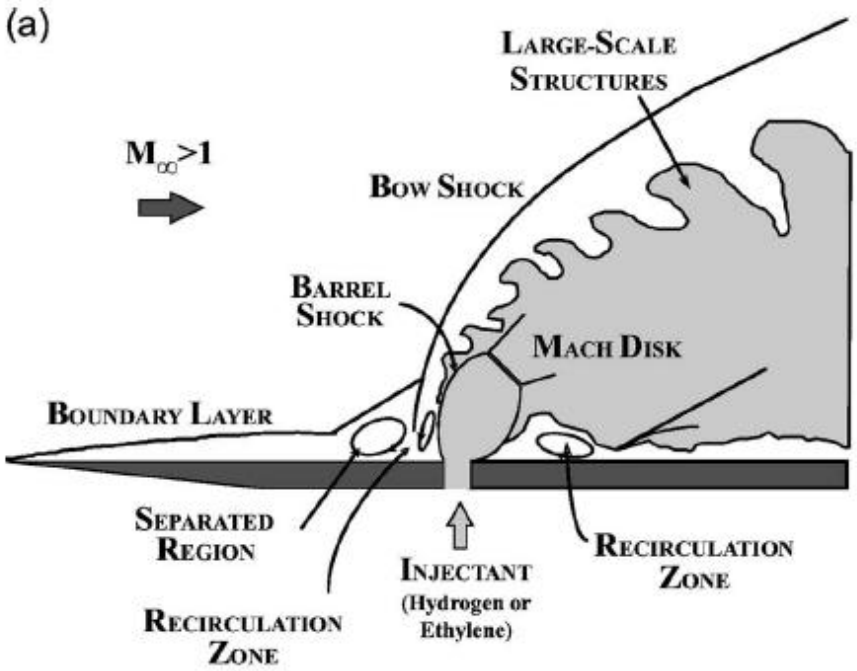
Skin friction coefficient (C_f)

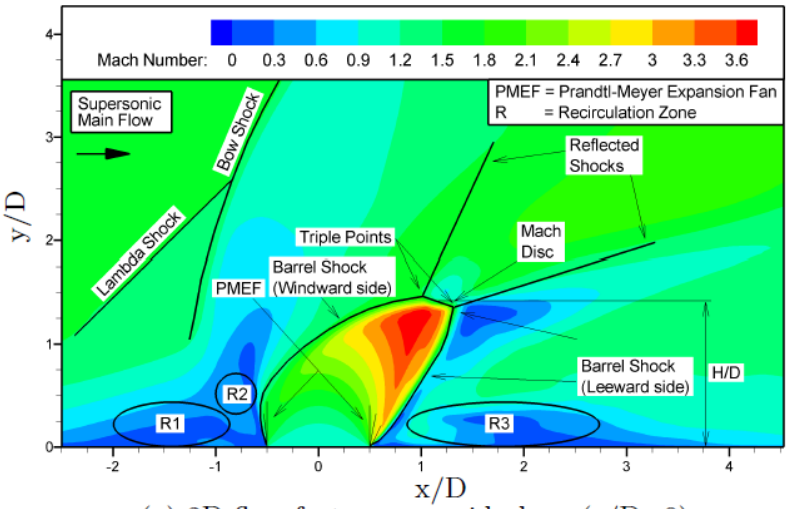


Wall pressure (P_{wall})

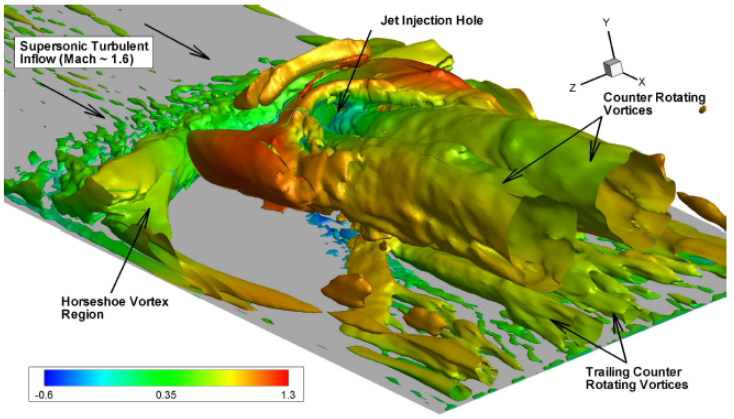
Sonic Transverse Jet in a Supersonic Cross-flow (JISC)

JISC was studied experimentally to understand the effects of the injection of a sonic circular jet on a supersonic cross-flow transversely.





(a) 2D flow features on mid plane (z/D=0)



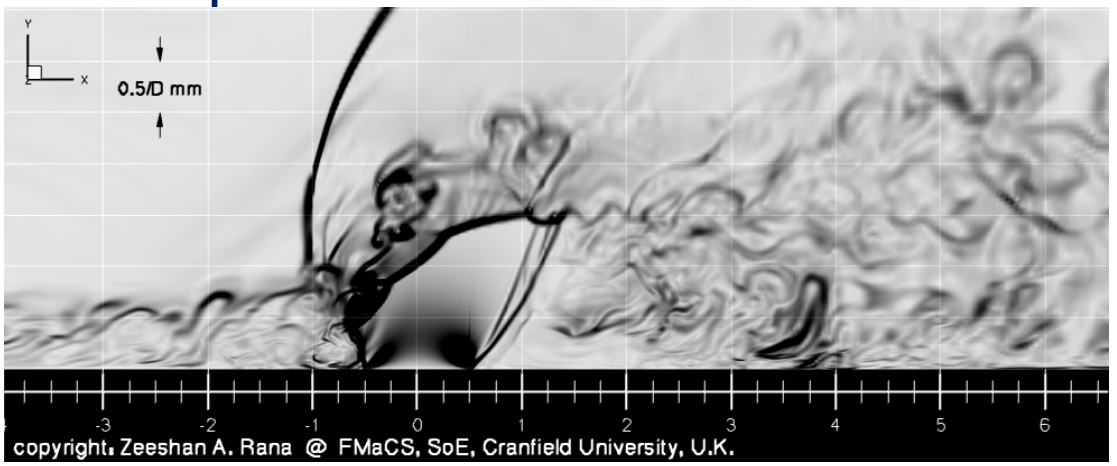
(b) 3D flow features; Q criterion Iso-Surfaces

JISC

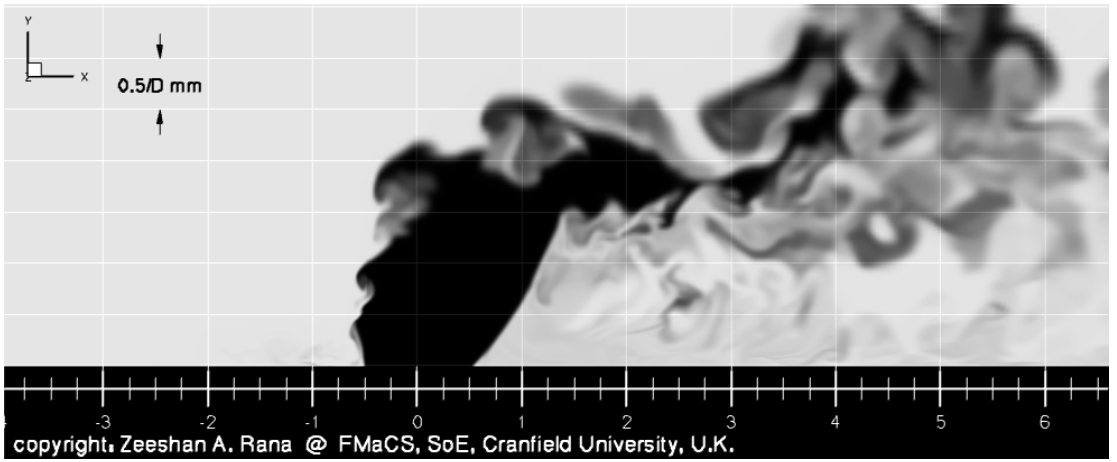
Results – Mach 1.6 JISC Experiment:

- Flow animations:

(a) Density Gradient,



(b) Passive Scalar



JISC

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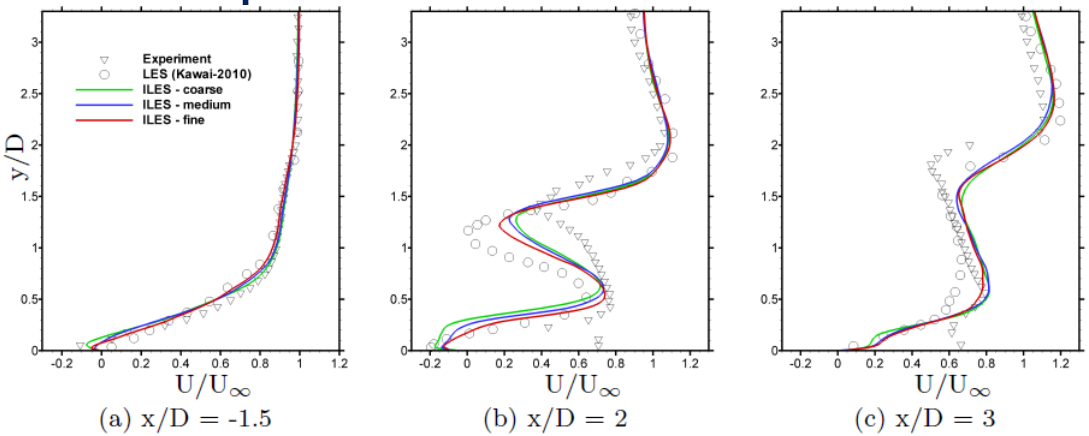
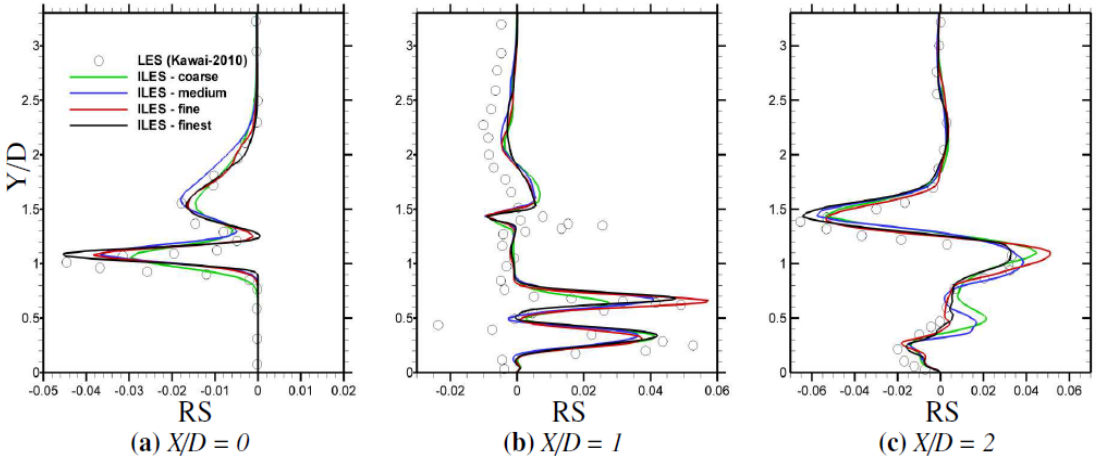
Results – Mach 1.6 JISC Experiment:

Streamwise Velocity Profile Comparison at mid-plane (z=0)



(a) x/D = -1.5 (b) x/D = 2 (c) x/D = 3

Turbulent Kinetic Energy Profile Comparison at mid-plane (z=0)

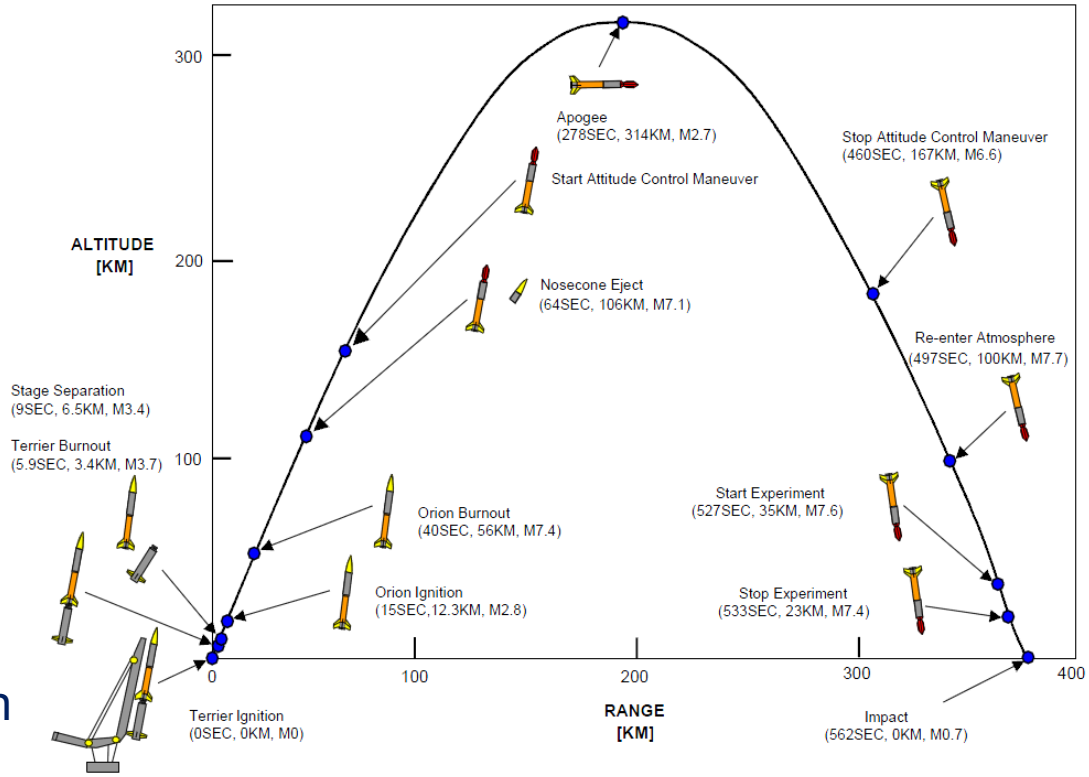


(a) *X/D = 0* **(b)** *X/D = 1* **(c)** *X/D = 2*

HyShot-II

HyShot-II Scramjet:

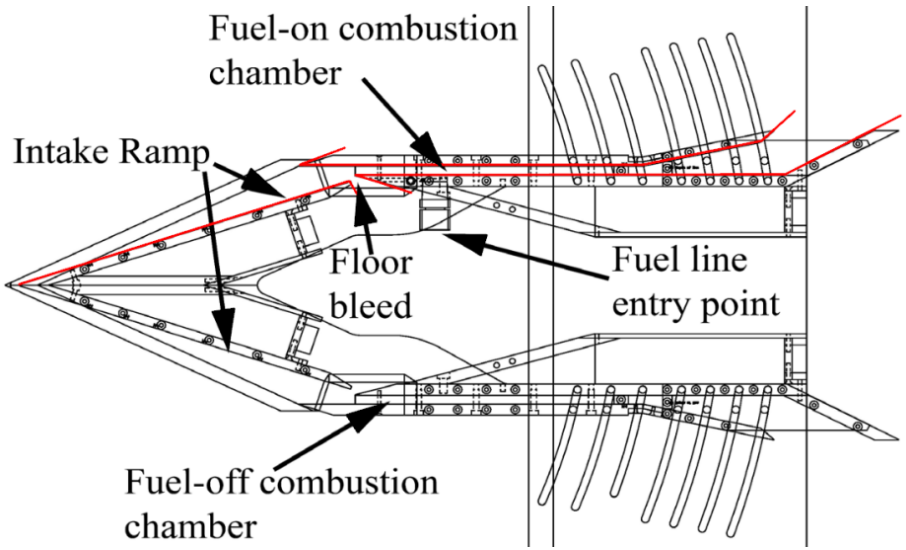
- Successful test flight – 30th July 2002
- Achieved Supersonic Combustion (SC) at Mach 7.6 at altitude of between 35 km and 23 km.
- Fuel - Gaseous Hydrogen
- Highly parabolic trajectory (near Vertical decent) to obtain correlations over a range of ambient pressures.

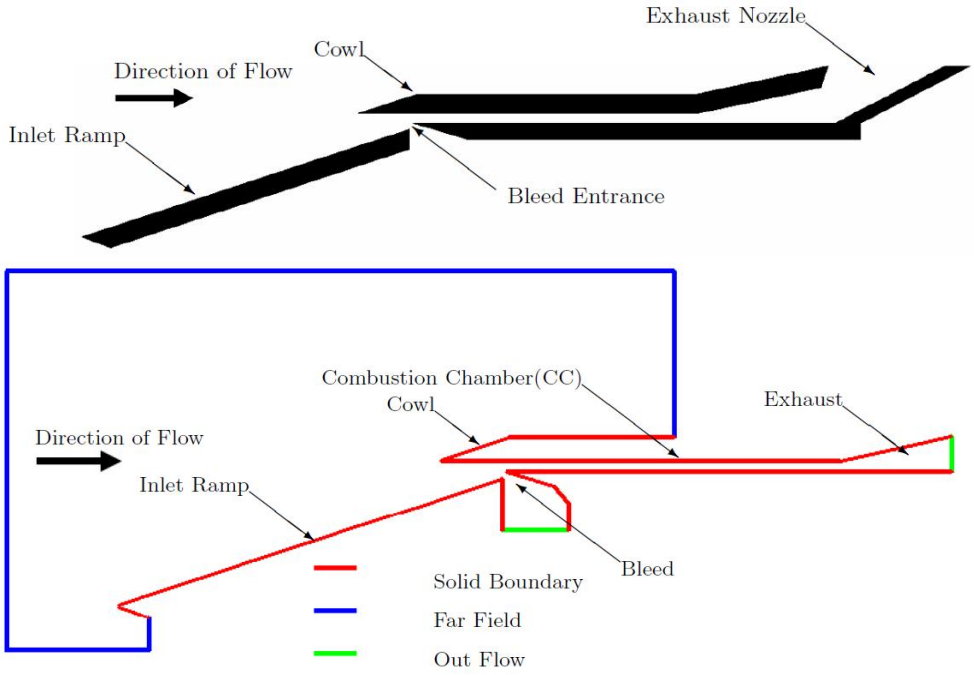


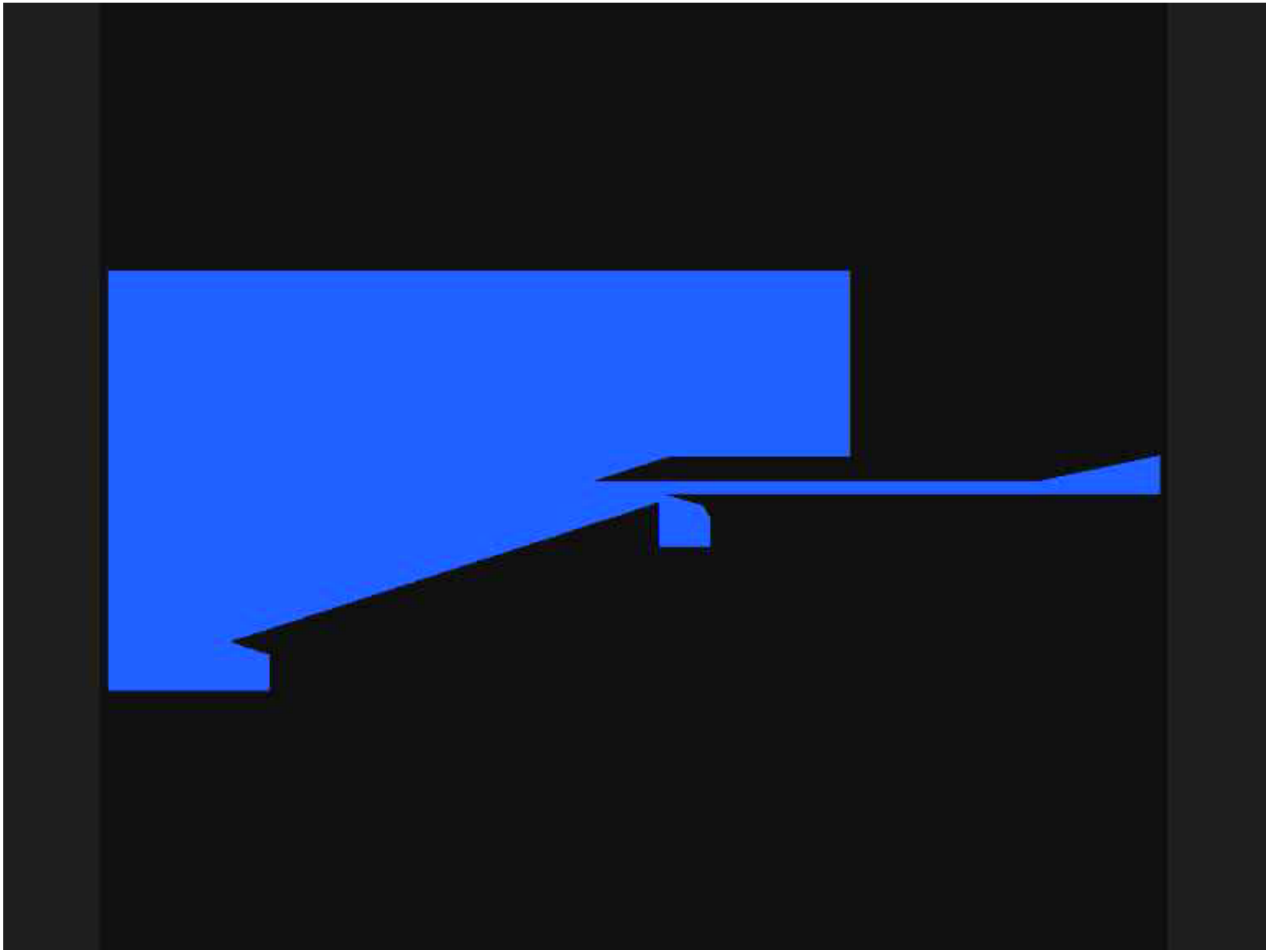
HyShot-II

Results – Analysis of the HyShot-II Scramjet:

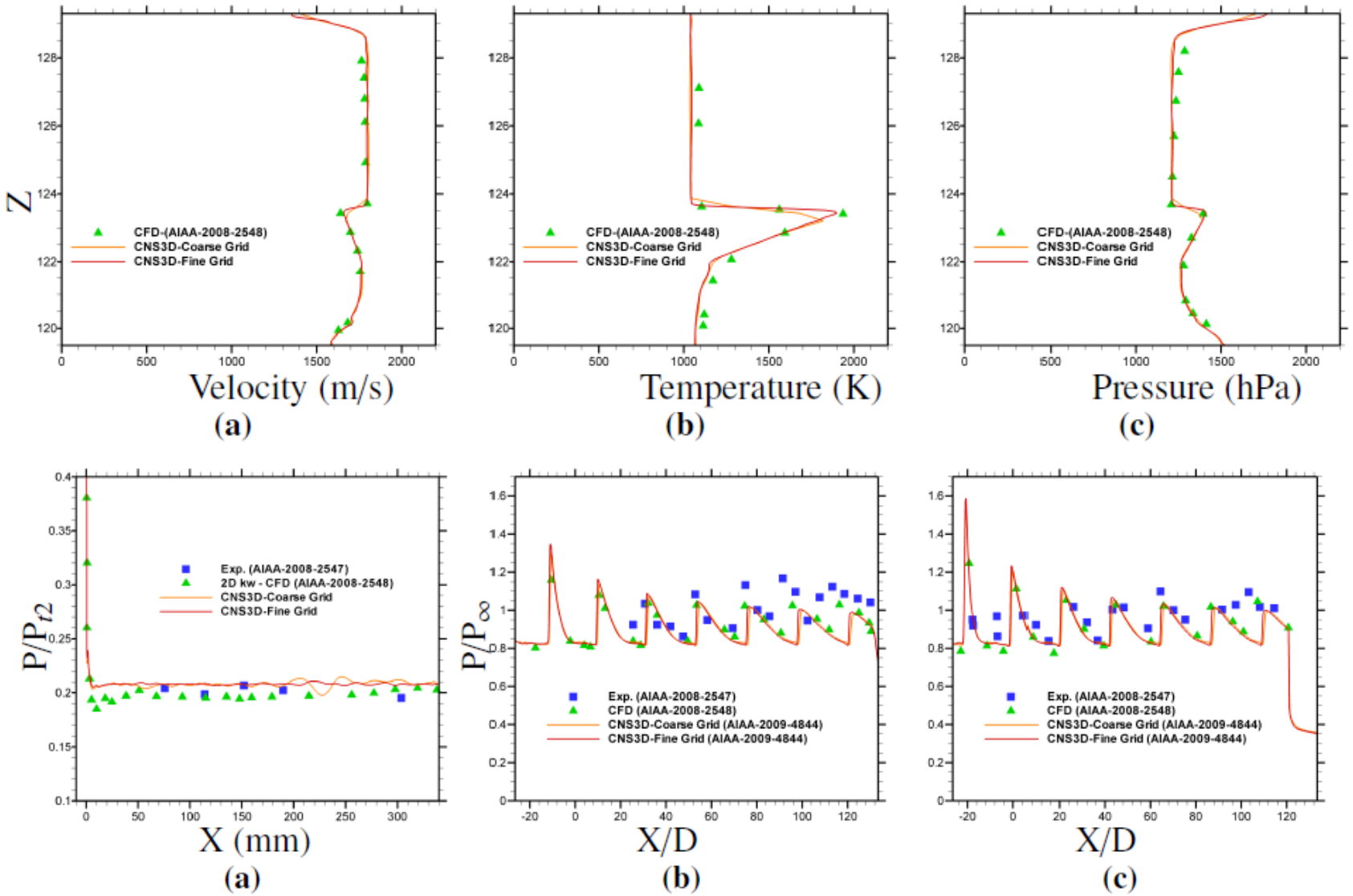
- Pressure measurements - the primary means for obtaining the correlation
- Combustion and non-combustion investigations on the geometry are carried out at DLR, Germany using HEG and CFD.





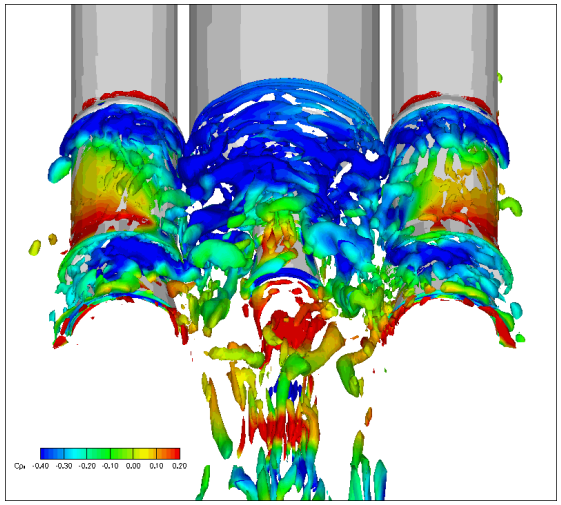


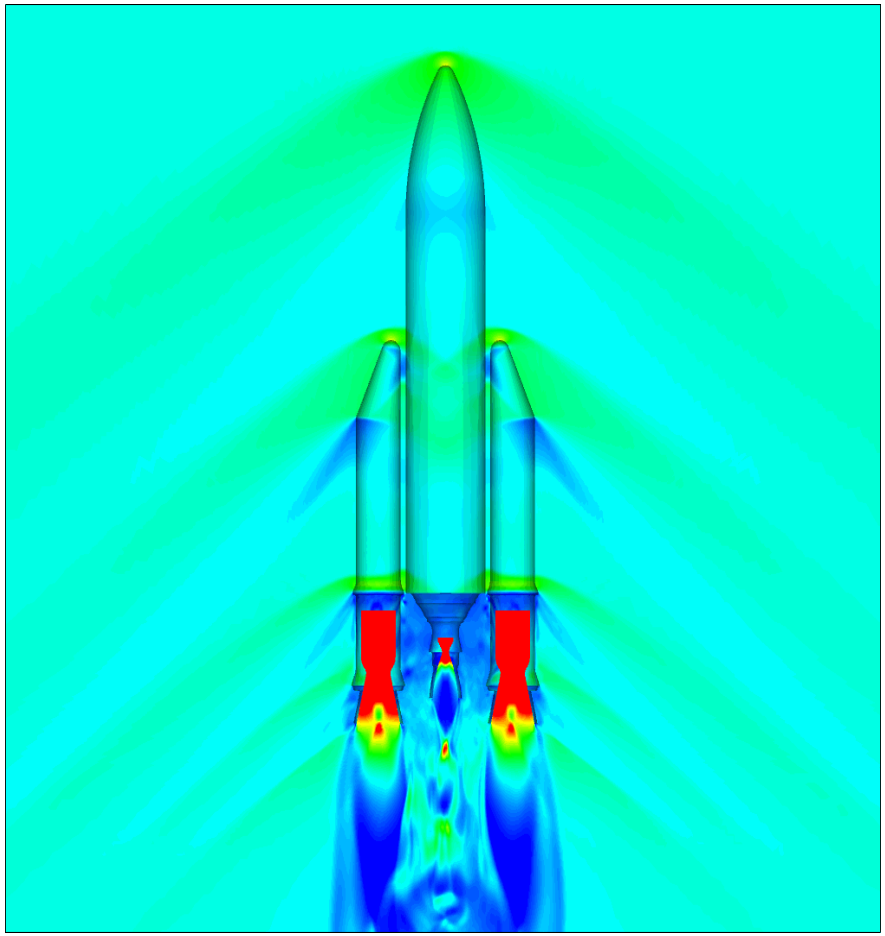
HyShot-II


Z
CFD-(AIAA-2008-2548)
CNS3D-Coarse Grid
CNS3D-Fine Grid
Velocity (m/s)
(a)
Temperature (K)
(b)
Pressure (hPa)
(c)
P/Pt2
Exp. (AIAA-2008-2547)
2D kw - CFD (AIAA-2008-2548)
CNS3D-Coarse Grid
CNS3D-Fine Grid
X (mm)
(a)
P/P∞
Exp. (AIAA-2008-2547)
CFD (AIAA-2008-2548)
CNS3D-Coarse Grid (AIAA-2009-4844)
CNS3D-Fine Grid (AIAA-2009-4844)
X/D
(b)
X/D
(c)

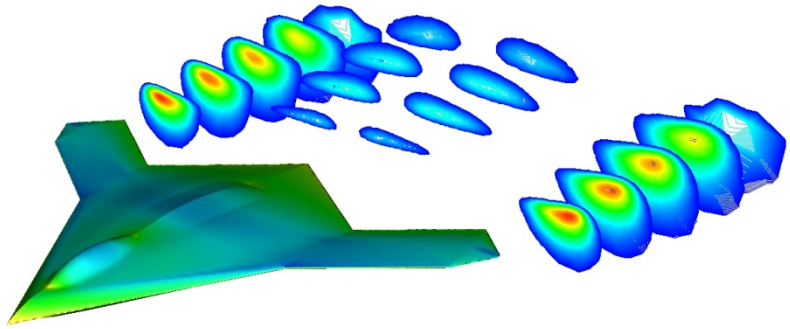
Launcher Aerodynamics

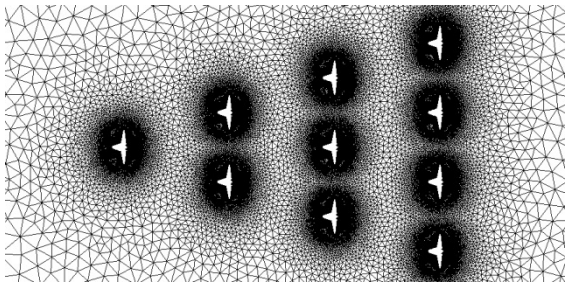
- Ariane nozzles experience high side loadings due to vortex shedding
- Can cause serious control issues and
- Limit the development of combustion chambers as longer nozzles cannot be employed

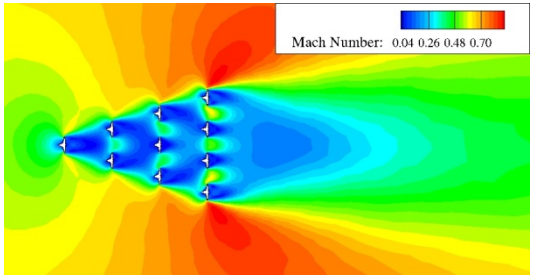


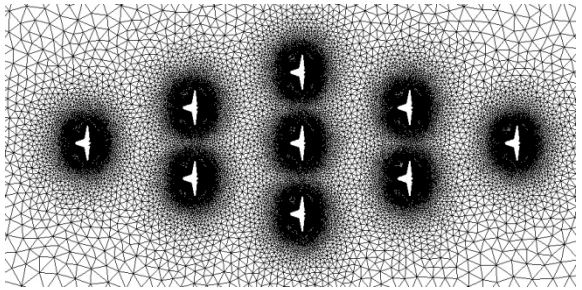


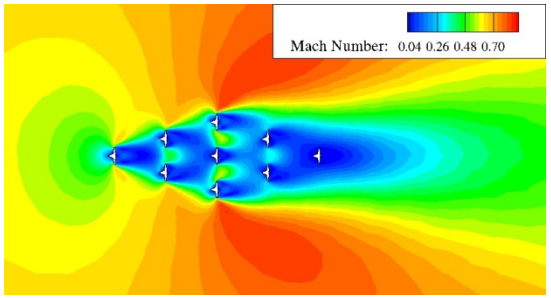
UAV flying formation

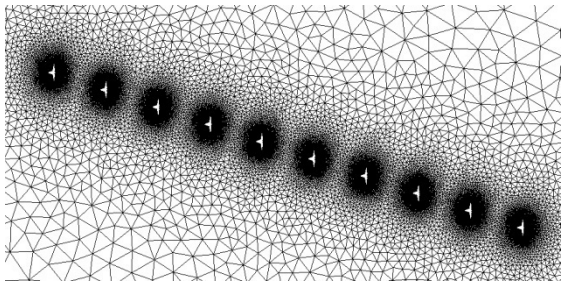


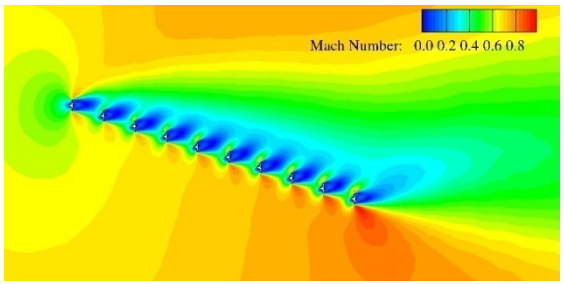


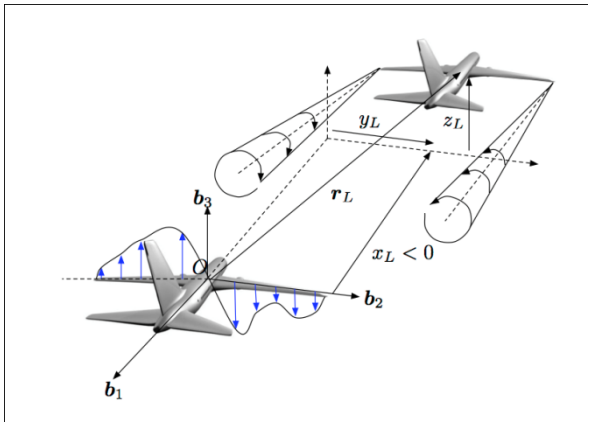


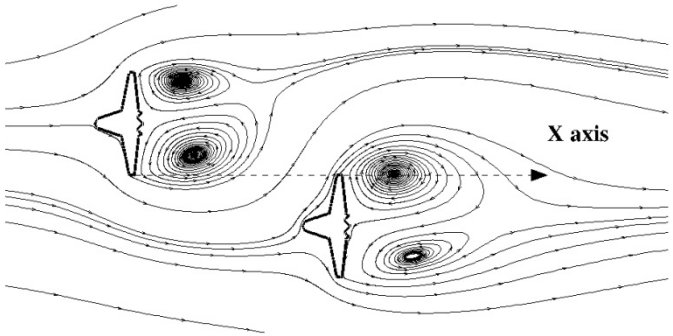






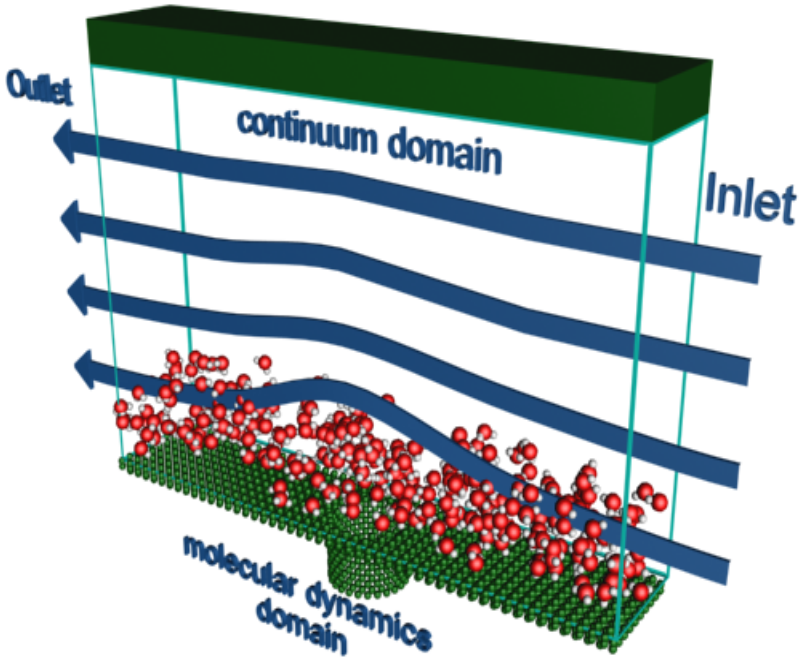






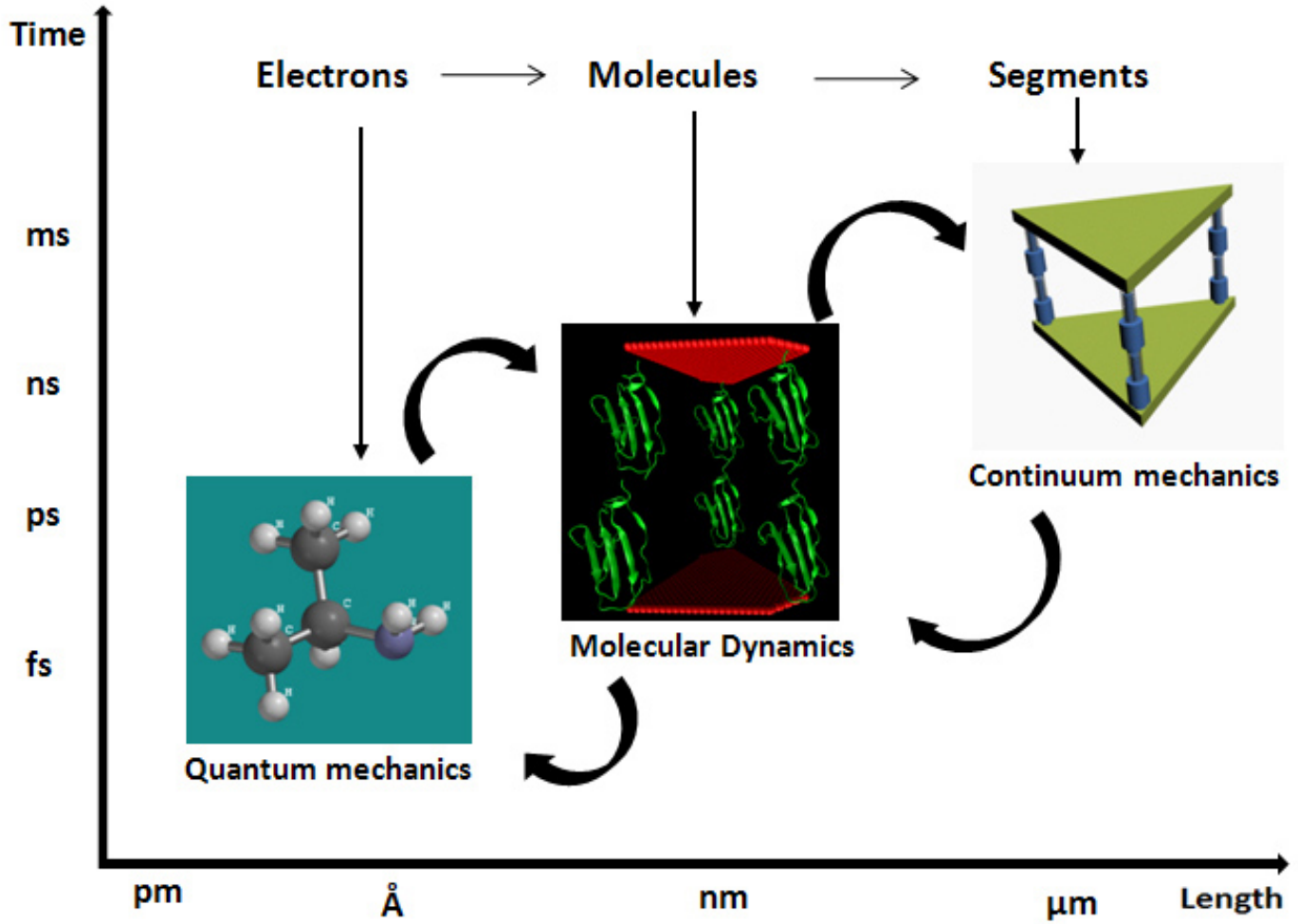
From Macro to Nano Scale

- Several new applications and design concepts require understanding of fluid/material phenomena and interactions at micro and nano scale.
- This motivates the design of multi-scale methods
- Multi-scale modelling and simulations can also be used in support of the development of simpler engineering models.



Example of coupling flow, near-wall molecular transport, and solid material

Molecular and Multi-Scale methods



Molecular Dynamics

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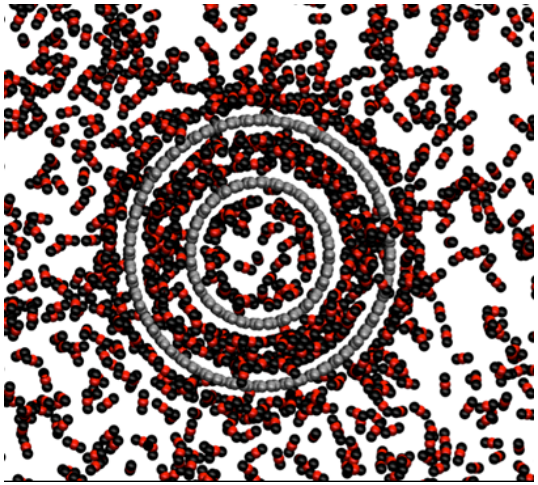
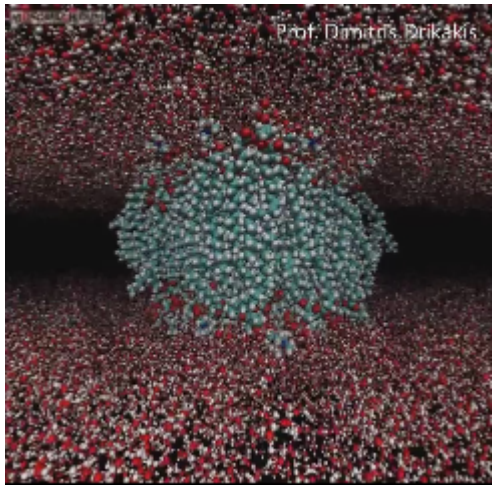
Effective for studying confined fluids

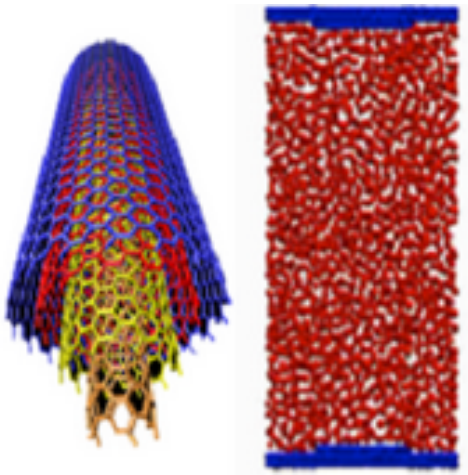
- Investigate interface effects from first principles
- Level of detail beyond experimental possibilities



Challenges

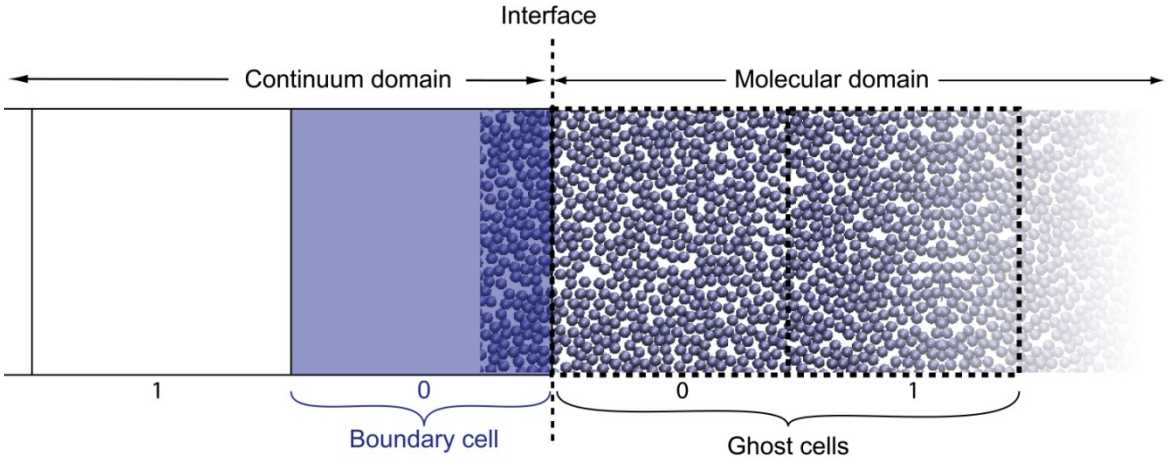
- Difficult to accurately model complex physical systems
- Complications in extracting macroscopic properties from phase space trajectories
- Computational expense



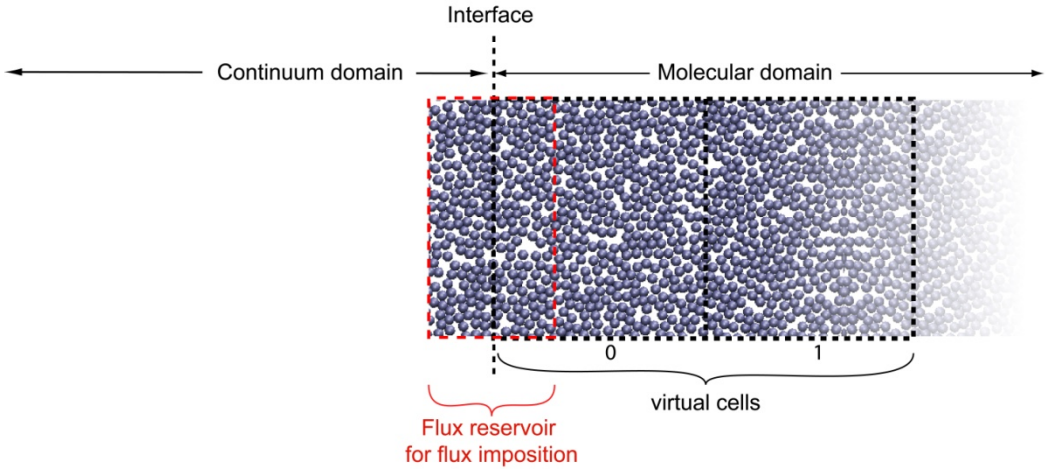


Hybrid solution interface

Continuum perspective



Molecular perspective



Point-wise coupling

- Continuum covers the entire domain
- MD solver is used as a local refinement to replace analytical or empirical models
- Two types of relations:

  Constitutive relations:

  – Compute equations of state, e.g., $p=p(r,\mathbf{c},T)$

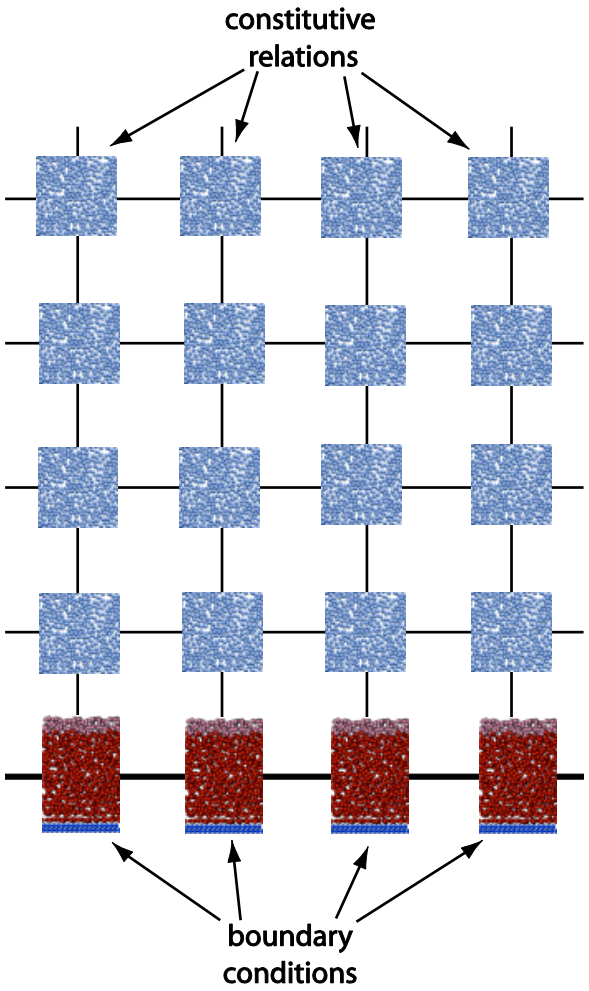
  – Compute transport coefficients, e.g., viscosity, diffusion coefficient, heat conductivity

  Boundary conditions:

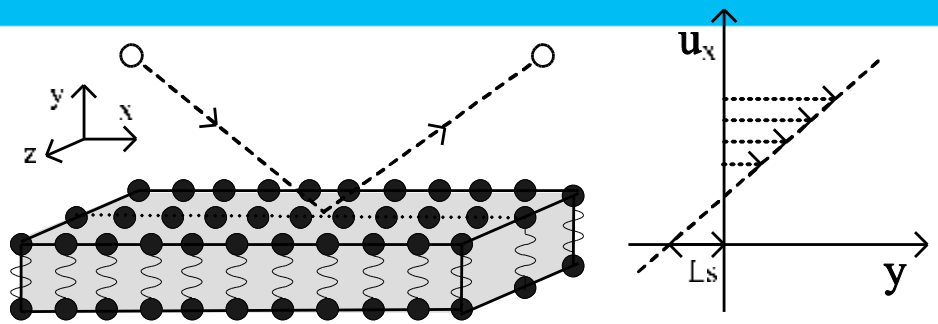
  – Tangentrial stress $t_t= t_t(r,\mathbf{c},T,u)$,

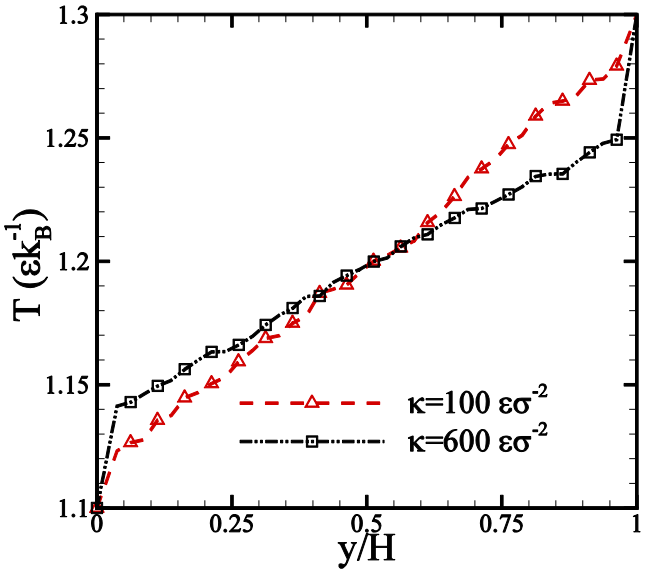
  – Heat flux, $q=q(r,\mathbf{c},T,u)$

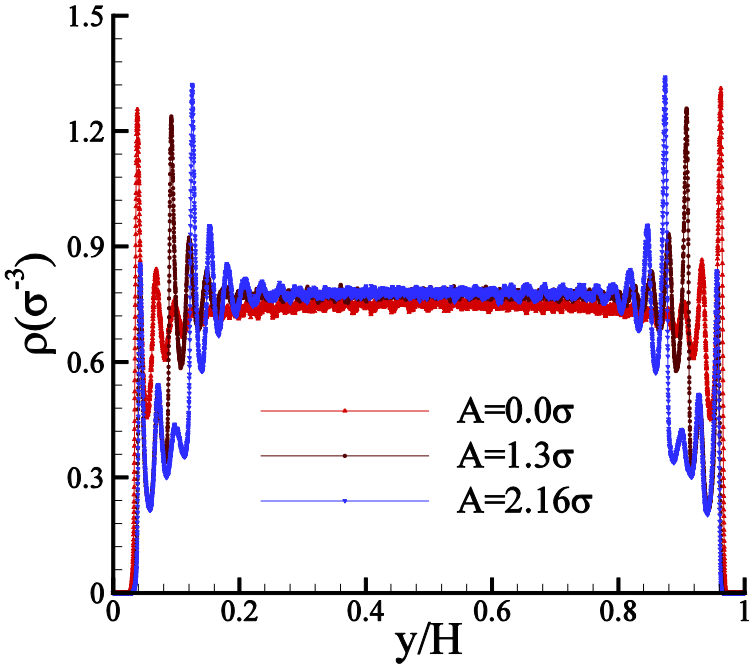
  – slip velocity, $v_s=v_s(r,\mathbf{c},T,u)$,



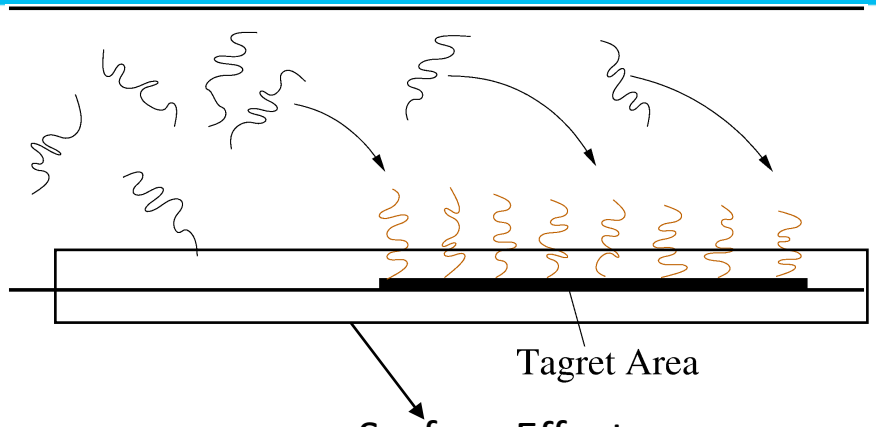
Modelling surface effects



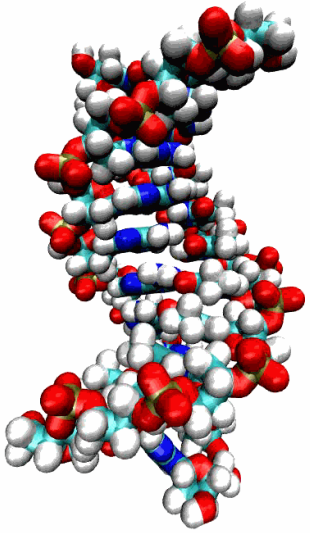


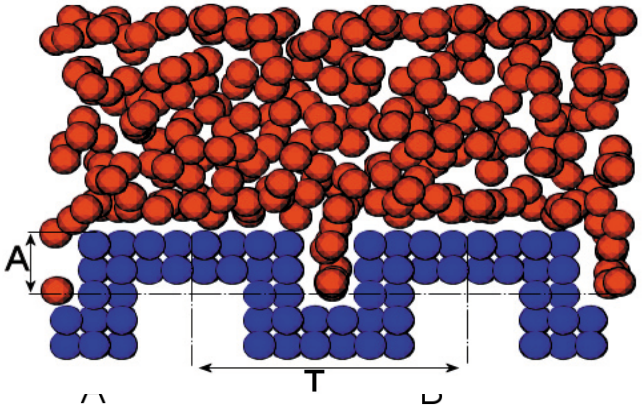


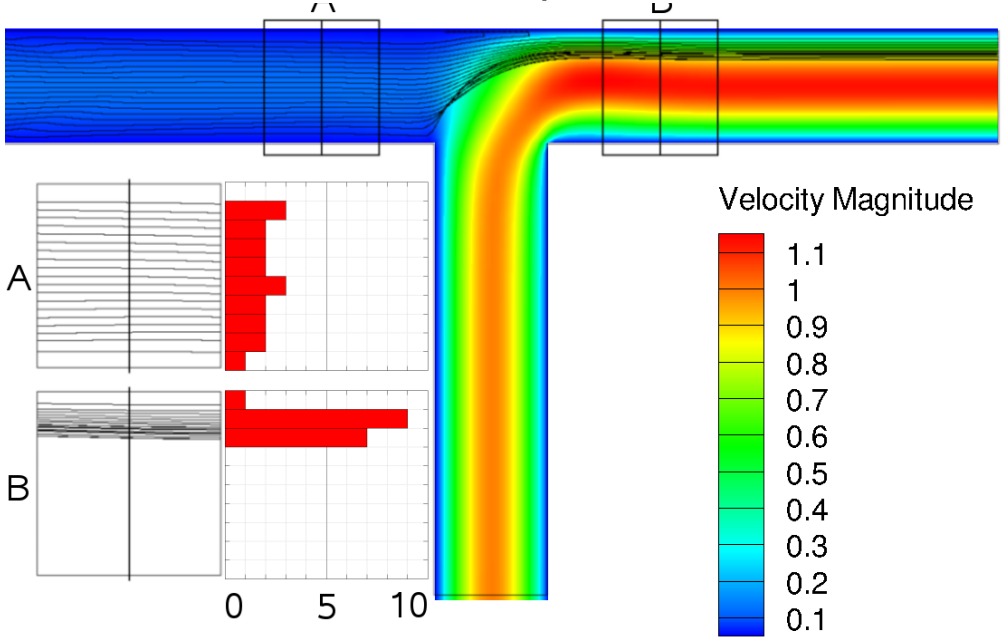
DNA transport in micro-fluidics



Surface Effects







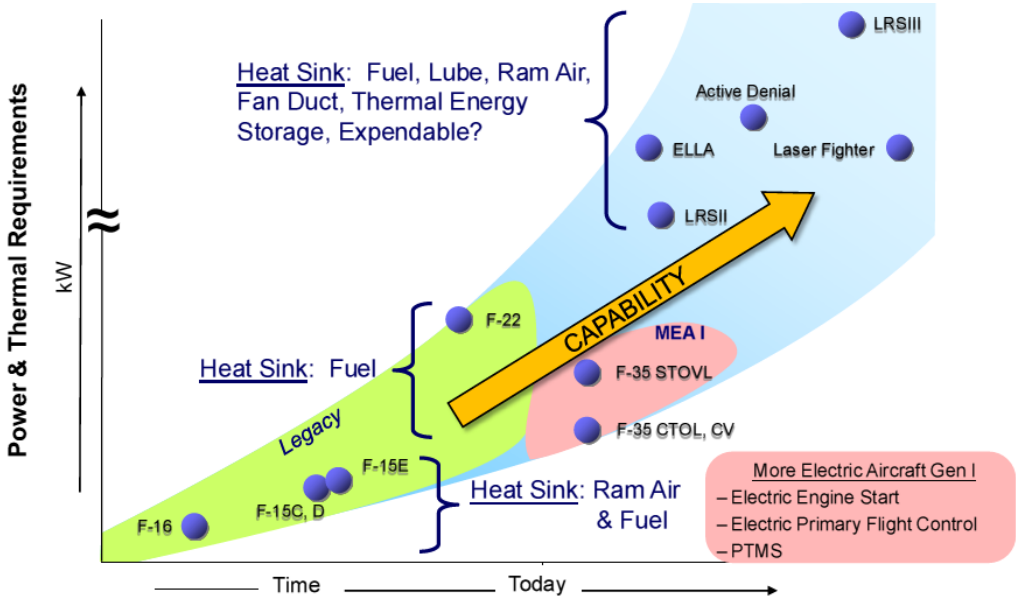
Thermal Management

Important problem in avionics

- Heat fluxes of the order of 10^3 W/cm^2
- Failures during flight
- Limiting factor for additional functionality

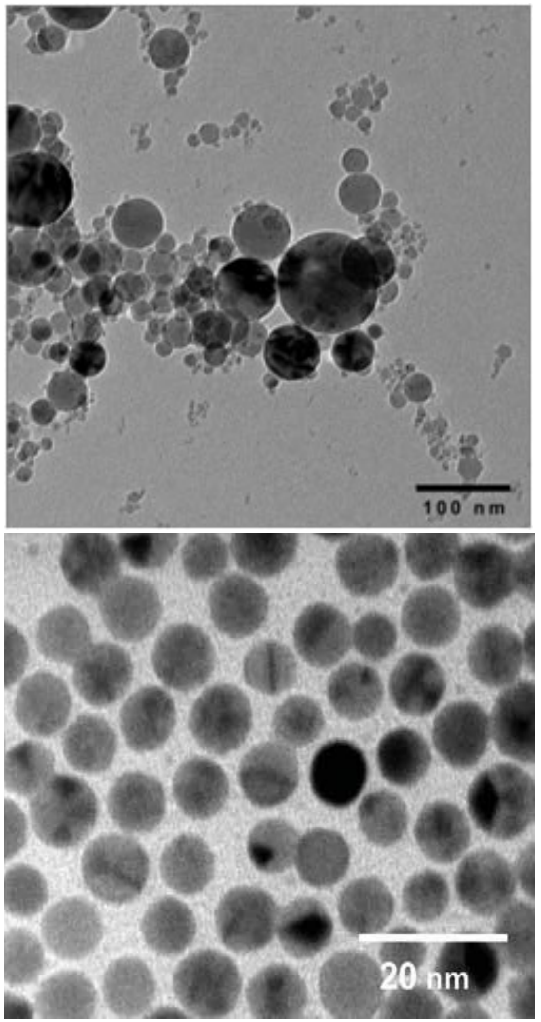
Cause

- Low thermal conductivity conventional materials
- Liquid cooling has reached its limits



Nanofluids

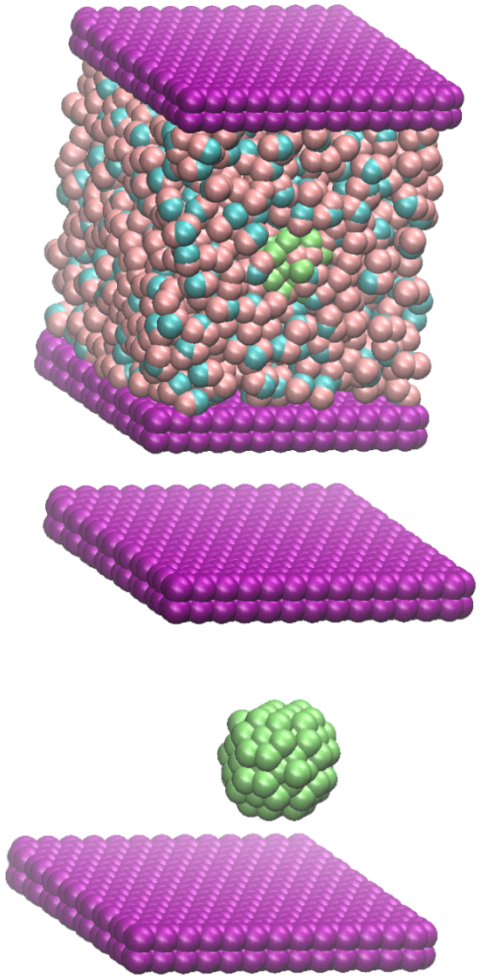
- Suspensions of solid particles with nanometer size diameters in a fluid
- Nanofluids have enhanced thermal properties
- Physical explanation and theoretical models are a topic of debate



Nanofluid

Water-Copper nanofluid, confined in graphene walls

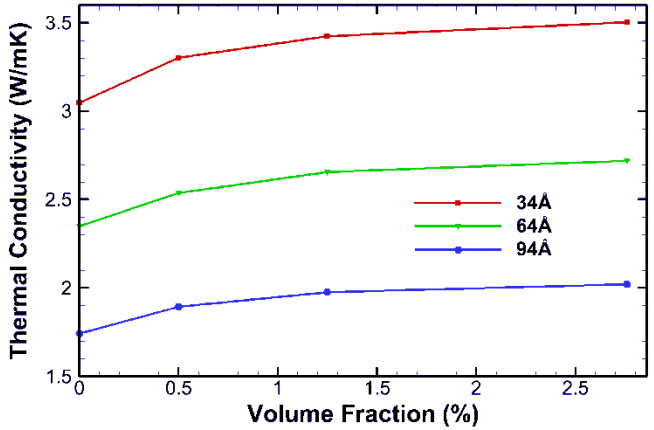
- Thermal conductivity was calculated for various wall separation distances for different volume fractions.

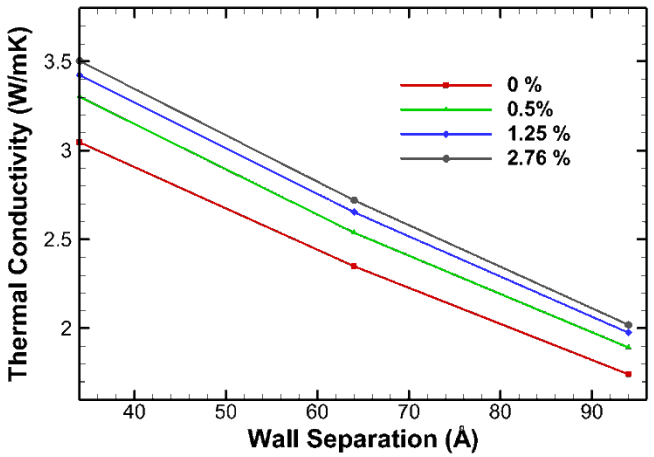


Nanofluid

Thermal conductivity

- Increases with increasing volume fraction
- All curves have similar shape
- As the wall separation distance decreases, the thermal conductivity for all particle loadings experiences a jump

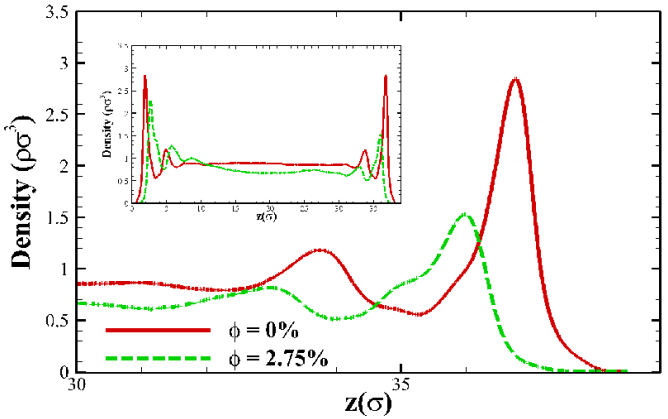




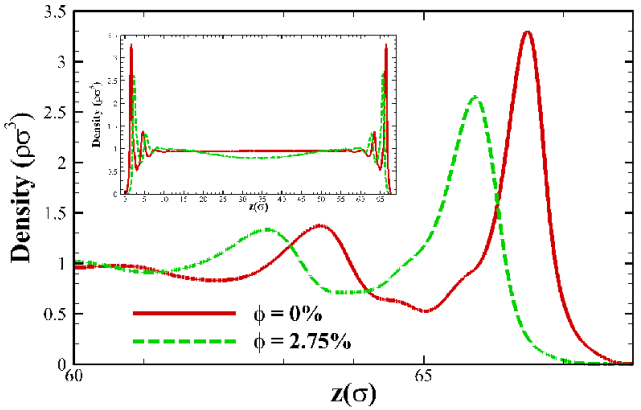
Nanofluid

Particle affects structure of liquid atoms

- Graphene is hydrophobic
- Addition of particle attracts the density layers at the solid/liquid interface
- The smaller the channel is the more effect the particle has to the solid-liquid interface
- In turn the thermal conductivity is affected



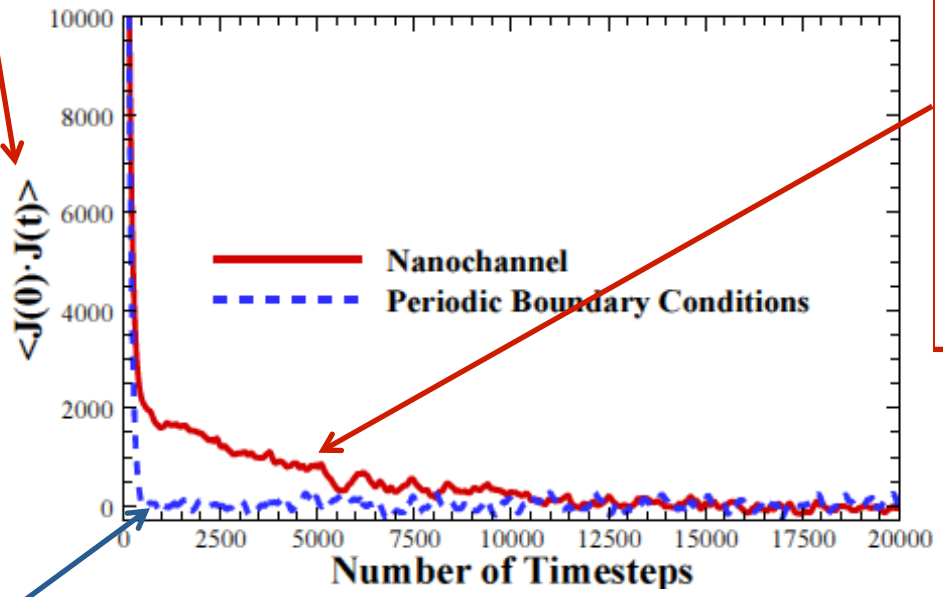
34Å Channel width



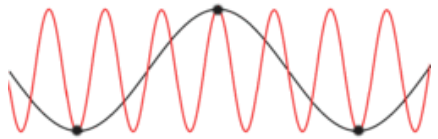
94Å Channel width

Ballistic heat transfer

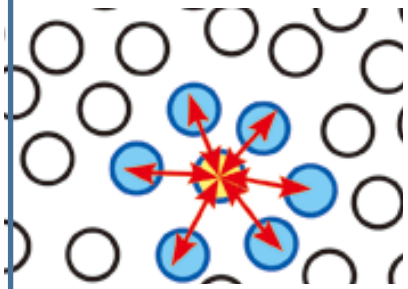
$$\lambda = \frac{1}{3k_B VT^2}\int_0^t \langle q(0)\cdot q(t)\rangle dt$$



Ballistic heat transfer



Diffusive heat transfer



Concluding remarks

- High-order CFD has significant potential for addressing design challenges
- MD and multi-scale modelling can provide new insights into small scale phenomena that can enable the development of new technologies.
- Hybrid molecular-continuum methods for solids and fluids are capable of resolving physics on micro/nano scale
- Research into the development of more accurate and efficient methods as well as software redesign need to go hand-in-hand with the High Performance Computing advancements